



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:39 PM UTC

PDB ID : 2PDA / pdb\_00002pda  
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN PYRUVATE-FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIBRIO AFRICANUS AND PYRUVATE.  
Authors : Chabriere, E.; Charon, M.H.  
Deposited on : 1998-11-10  
Resolution : 3.00 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

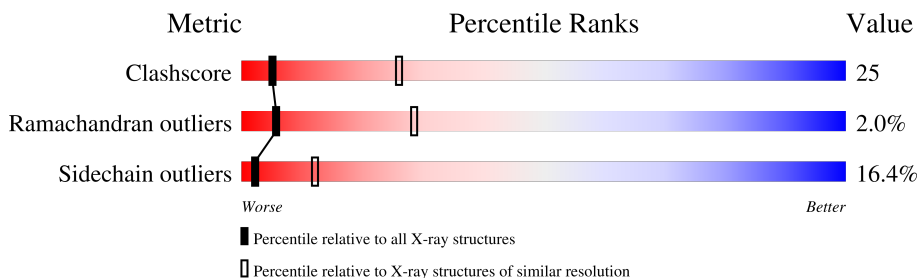
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1231	50% 38% 11% .
1	B	1231	50% 38% 11% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	A	1234	-	-	X	-
4	SF4	B	1241	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18894 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 PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	25	0	0
			9382	5941	1599	1783	59			
1	B	1231	Total	C	N	O	S	25	0	0
			9382	5941	1599	1783	59			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0
4	A	1	Total Fe S 8 4 4	0	0
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



- Molecule 7 is water.

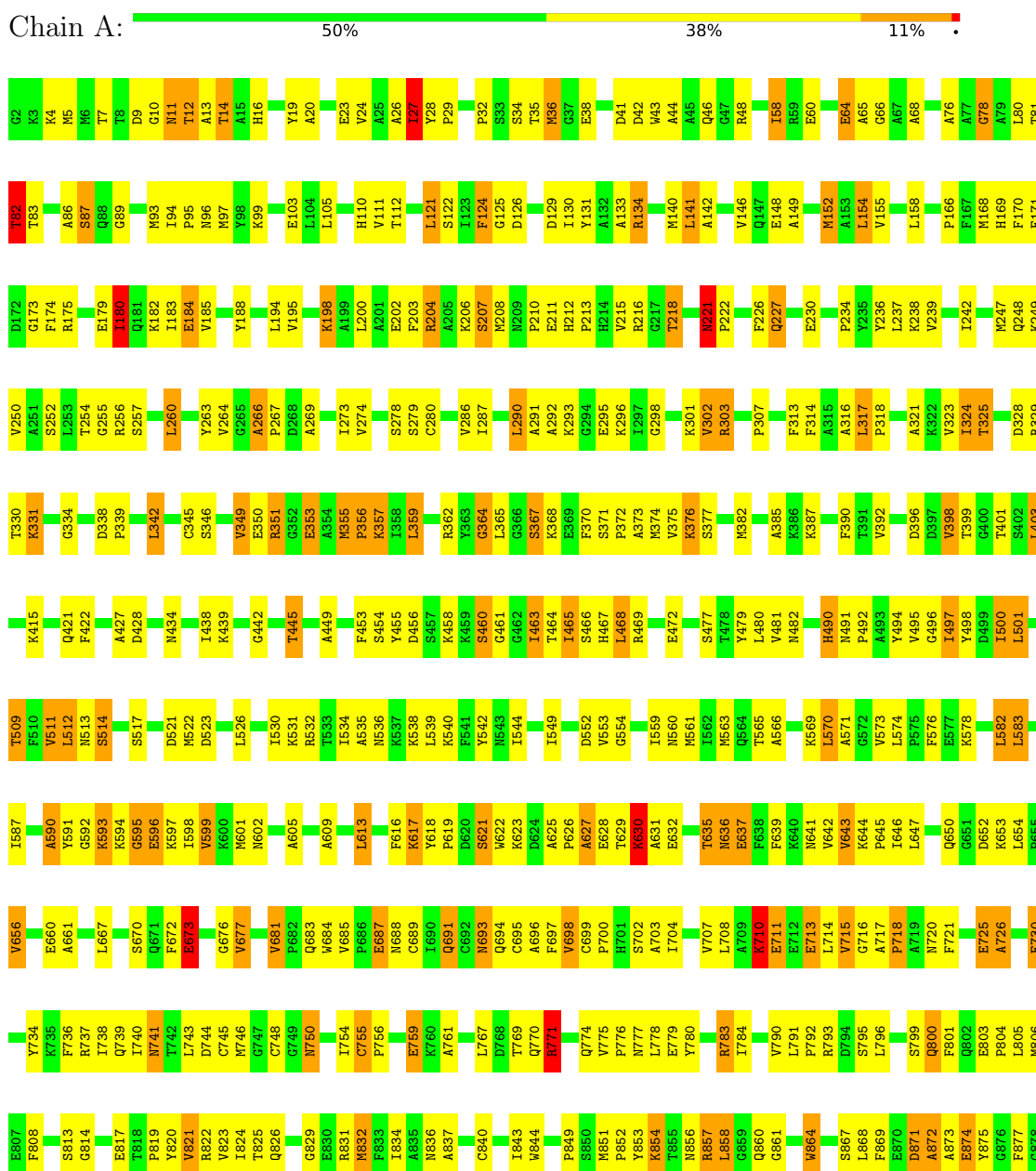
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O 7 7	0	0
7	B	7	Total O 7 7	0	0

### 3 Residue-property plots

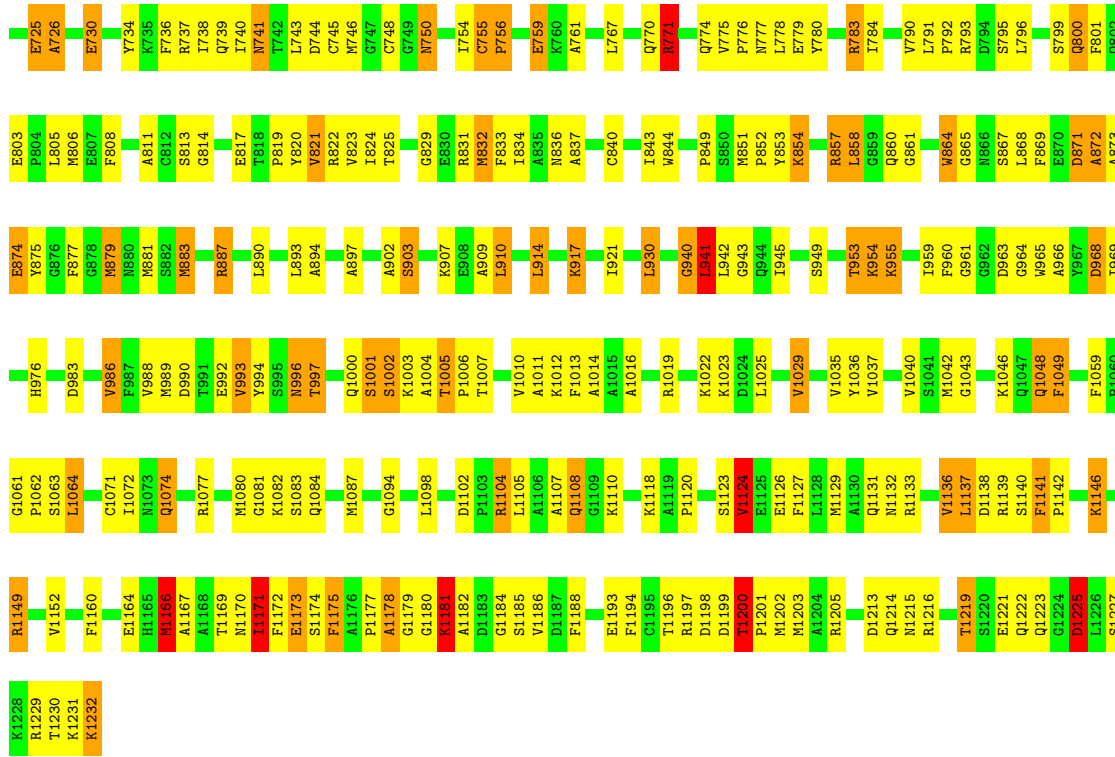
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.00Å 146.30Å 211.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.2 (10.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR 3.854	Depositor
R, $R_{free}$	0.234 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	18894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PYR, TPP, CA, SF4

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	0.85	7/9584 (0.1%)	1.30	116/12954 (0.9%)
1	B	0.85	7/9584 (0.1%)	1.30	115/12954 (0.9%)
All	All	0.85	14/19168 (0.1%)	1.30	231/25908 (0.9%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	879	MET	SD-CE	-6.70	1.62	1.79
1	A	879	MET	SD-CE	-6.68	1.62	1.79
1	A	953	THR	CA-CB	6.13	1.62	1.53
1	B	953	THR	CA-CB	6.11	1.62	1.53
1	A	36	MET	SD-CE	-5.86	1.64	1.79
1	B	36	MET	SD-CE	-5.84	1.65	1.79
1	B	94	ILE	CA-CB	5.65	1.57	1.54
1	A	94	ILE	CA-CB	5.57	1.57	1.54
1	A	872	ALA	CA-CB	-5.53	1.44	1.53
1	B	872	ALA	CA-CB	-5.52	1.44	1.53
1	A	180	ILE	CA-CB	5.15	1.60	1.54
1	B	180	ILE	CA-CB	5.12	1.60	1.54
1	B	302	VAL	CA-CB	5.08	1.61	1.54
1	A	302	VAL	CA-CB	5.08	1.61	1.54

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	497	ILE	N-CA-C	13.25	125.44	111.00
1	A	497	ILE	N-CA-C	13.25	125.44	111.00
1	B	592	GLY	N-CA-C	-10.99	99.05	115.32
1	A	592	GLY	N-CA-C	-10.96	99.09	115.32
1	B	756	PRO	N-CA-C	10.96	124.08	110.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	756	PRO	N-CA-C	10.93	124.04	110.70
1	A	755	CYS	CA-C-N	10.23	130.91	120.38
1	A	755	CYS	C-N-CA	10.23	130.91	120.38
1	B	755	CYS	CA-C-N	10.18	130.87	120.38
1	B	755	CYS	C-N-CA	10.18	130.87	120.38
1	B	590	ALA	N-CA-C	-9.92	97.43	110.53
1	A	590	ALA	N-CA-C	-9.90	97.47	110.53
1	B	1005	THR	CA-C-N	8.88	128.83	120.03
1	B	1005	THR	C-N-CA	8.88	128.83	120.03
1	A	1005	THR	CA-C-N	8.88	128.82	120.03
1	A	1005	THR	C-N-CA	8.88	128.82	120.03
1	A	27	ILE	N-CA-C	8.61	121.38	108.80
1	B	27	ILE	N-CA-C	8.60	121.35	108.80
1	B	625	ALA	N-CA-C	-8.21	99.40	109.83
1	A	625	ALA	N-CA-C	-8.17	99.45	109.83
1	B	871	ASP	N-CA-C	8.14	121.30	110.88
1	A	871	ASP	N-CA-C	8.12	121.28	110.88
1	A	636	ASN	N-CA-C	8.08	120.76	110.33
1	B	65	ALA	N-CA-C	-8.07	101.23	112.45
1	A	65	ALA	N-CA-C	-8.07	101.24	112.45
1	B	636	ASN	N-CA-C	8.06	120.73	110.33
1	B	618	TYR	CA-C-N	7.92	127.92	119.76
1	B	618	TYR	C-N-CA	7.92	127.92	119.76
1	A	618	TYR	CA-C-N	7.90	127.90	119.76
1	A	618	TYR	C-N-CA	7.90	127.90	119.76
1	A	1166	MET	N-CA-C	-7.68	94.45	110.80
1	B	1166	MET	N-CA-C	-7.67	94.45	110.80
1	A	641	ASN	N-CA-C	7.62	122.68	113.23
1	B	641	ASN	N-CA-C	7.62	122.67	113.23
1	B	1061	GLY	CA-C-N	7.54	127.55	119.78
1	B	1061	GLY	C-N-CA	7.54	127.55	119.78
1	A	1061	GLY	CA-C-N	7.53	127.54	119.78
1	A	1061	GLY	C-N-CA	7.53	127.54	119.78
1	A	355	MET	CA-C-N	7.44	129.14	119.84
1	A	355	MET	C-N-CA	7.44	129.14	119.84
1	B	355	MET	CA-C-N	7.44	129.14	119.84
1	B	355	MET	C-N-CA	7.44	129.14	119.84
1	B	125	GLY	N-CA-C	7.40	125.74	111.31
1	A	125	GLY	N-CA-C	7.40	125.74	111.31
1	B	909	ALA	N-CA-C	-7.38	102.83	111.03
1	A	909	ALA	N-CA-C	-7.36	102.86	111.03
1	B	203	PHE	N-CA-C	-7.29	103.34	111.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	PHE	N-CA-C	-7.29	103.34	111.28
1	A	635	THR	N-CA-C	-7.18	98.10	109.23
1	B	635	THR	N-CA-C	-7.16	98.13	109.23
1	B	559	ILE	N-CA-C	7.13	121.81	112.76
1	A	877	PHE	N-CA-C	-7.13	104.39	113.23
1	A	559	ILE	N-CA-C	7.11	121.78	112.76
1	B	877	PHE	N-CA-C	-7.10	104.43	113.23
1	A	26	ALA	N-CA-C	-7.10	97.67	109.24
1	B	26	ALA	N-CA-C	-7.07	97.72	109.24
1	A	560	ASN	N-CA-C	7.04	119.55	111.11
1	B	560	ASN	N-CA-C	7.03	119.55	111.11
1	B	627	ALA	N-CA-C	7.03	125.77	110.80
1	A	627	ALA	N-CA-C	7.00	125.72	110.80
1	B	1200	THR	CA-C-N	6.95	127.09	119.87
1	B	1200	THR	C-N-CA	6.95	127.09	119.87
1	A	1200	THR	CA-C-N	6.93	127.08	119.87
1	A	1200	THR	C-N-CA	6.93	127.08	119.87
1	B	1014	ALA	N-CA-C	-6.91	102.45	111.71
1	A	625	ALA	CA-C-N	-6.91	111.20	119.84
1	A	625	ALA	C-N-CA	-6.91	111.20	119.84
1	A	1014	ALA	N-CA-C	-6.91	102.46	111.71
1	A	207	SER	N-CA-C	6.89	118.88	110.41
1	B	16	HIS	N-CA-C	-6.89	103.46	110.97
1	B	207	SER	N-CA-C	6.88	118.88	110.41
1	A	711	GLU	N-CA-C	6.88	125.45	110.80
1	A	16	HIS	N-CA-C	-6.87	103.48	110.97
1	B	625	ALA	CA-C-N	-6.87	111.25	119.84
1	B	625	ALA	C-N-CA	-6.87	111.25	119.84
1	B	711	GLU	N-CA-C	6.86	125.41	110.80
1	B	195	VAL	N-CA-C	6.79	117.80	108.84
1	A	195	VAL	N-CA-C	6.78	117.80	108.84
1	B	124	PHE	N-CA-C	6.76	118.58	110.19
1	A	124	PHE	N-CA-C	6.75	118.56	110.19
1	B	221	ASN	CA-C-N	-6.75	112.83	119.64
1	B	221	ASN	C-N-CA	-6.75	112.83	119.64
1	B	1175	PHE	N-CA-C	6.74	120.27	108.75
1	A	1175	PHE	N-CA-C	6.73	120.26	108.75
1	A	221	ASN	CA-C-N	-6.71	112.86	119.64
1	A	221	ASN	C-N-CA	-6.71	112.86	119.64
1	A	824	ILE	N-CA-C	-6.64	104.01	110.72
1	B	824	ILE	N-CA-C	-6.64	104.02	110.72
1	A	685	VAL	CA-C-N	6.63	126.88	119.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	VAL	C-N-CA	6.63	126.88	119.32
1	B	685	VAL	CA-C-N	6.61	126.85	119.32
1	B	685	VAL	C-N-CA	6.61	126.85	119.32
1	B	247	MET	N-CA-C	-6.60	104.11	111.71
1	A	247	MET	N-CA-C	-6.60	104.12	111.71
1	B	1072	ILE	N-CA-C	-6.46	104.19	110.72
1	A	1072	ILE	N-CA-C	-6.45	104.21	110.72
1	A	1049	PHE	N-CA-C	-6.36	104.27	111.14
1	B	1049	PHE	N-CA-C	-6.32	104.31	111.14
1	B	759	GLU	N-CA-C	-6.32	96.87	107.99
1	A	759	GLU	N-CA-C	-6.31	96.88	107.99
1	A	66	GLY	N-CA-C	-6.31	105.18	112.50
1	B	66	GLY	N-CA-C	-6.29	105.20	112.50
1	B	29	PRO	N-CA-C	6.25	120.31	110.50
1	A	29	PRO	N-CA-C	6.20	120.24	110.50
1	A	1140	SER	N-CA-C	6.17	120.81	113.28
1	B	1140	SER	N-CA-C	6.15	120.78	113.28
1	A	500	ILE	N-CA-C	6.15	117.63	110.62
1	B	500	ILE	N-CA-C	6.14	117.62	110.62
1	A	637	GLU	N-CA-C	-6.13	104.66	111.71
1	B	637	GLU	N-CA-C	-6.13	104.66	111.71
1	B	708	LEU	N-CA-C	-6.12	97.22	107.80
1	A	708	LEU	N-CA-C	-6.11	97.22	107.80
1	A	364	GLY	N-CA-C	6.06	127.55	113.18
1	B	364	GLY	N-CA-C	6.06	127.54	113.18
1	B	376	LYS	N-CA-C	-6.03	104.70	111.28
1	A	376	LYS	N-CA-C	-6.00	104.74	111.28
1	A	501	LEU	N-CA-C	5.97	119.52	112.72
1	B	501	LEU	N-CA-C	5.95	119.51	112.72
1	A	618	TYR	N-CA-C	5.93	119.24	109.58
1	B	618	TYR	N-CA-C	5.90	119.20	109.58
1	A	1046	LYS	N-CA-C	-5.86	105.97	113.23
1	B	1046	LYS	N-CA-C	-5.84	105.99	113.23
1	A	832	MET	N-CA-C	5.81	119.01	109.72
1	B	832	MET	N-CA-C	5.79	118.99	109.72
1	A	997	THR	N-CA-C	5.78	120.48	113.38
1	A	673	GLU	N-CA-C	5.76	118.43	111.40
1	B	997	THR	N-CA-C	5.76	120.47	113.38
1	B	673	GLU	N-CA-C	5.75	118.42	111.40
1	A	1081	GLY	N-CA-C	-5.73	105.69	113.37
1	A	861	GLY	CA-C-N	5.71	126.60	119.98
1	A	861	GLY	C-N-CA	5.71	126.60	119.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1081	GLY	N-CA-C	-5.70	105.73	113.37
1	B	1087	MET	N-CA-C	-5.70	105.06	111.28
1	B	861	GLY	CA-C-N	5.70	126.59	119.98
1	B	861	GLY	C-N-CA	5.70	126.59	119.98
1	B	630	LYS	N-CA-C	5.69	118.01	108.23
1	B	490	HIS	N-CA-C	5.68	119.91	113.15
1	A	1087	MET	N-CA-C	-5.68	105.09	111.28
1	A	630	LYS	N-CA-C	5.67	117.98	108.23
1	B	750	ASN	N-CA-C	5.66	117.91	111.11
1	A	750	ASN	N-CA-C	5.65	117.89	111.11
1	A	78	GLY	N-CA-C	5.65	121.80	115.08
1	B	78	GLY	N-CA-C	5.65	121.80	115.08
1	A	490	HIS	N-CA-C	5.65	119.87	113.15
1	B	385	ALA	N-CA-C	5.62	117.41	111.28
1	A	652	ASP	N-CA-C	-5.61	105.31	111.82
1	B	652	ASP	N-CA-C	-5.61	105.31	111.82
1	A	385	ALA	N-CA-C	5.61	117.39	111.28
1	B	13	ALA	N-CA-C	-5.59	105.19	111.28
1	A	983	ASP	N-CA-C	5.58	118.49	108.17
1	B	983	ASP	N-CA-C	5.58	118.49	108.17
1	A	13	ALA	N-CA-C	-5.56	105.22	111.28
1	A	313	PHE	N-CA-C	-5.55	104.92	110.97
1	B	1172	PHE	N-CA-C	5.54	116.88	108.07
1	B	313	PHE	N-CA-C	-5.53	104.94	110.97
1	A	1172	PHE	N-CA-C	5.52	116.85	108.07
1	B	631	ALA	N-CA-C	-5.52	100.62	109.39
1	A	631	ALA	N-CA-C	-5.51	100.62	109.39
1	B	255	GLY	N-CA-C	-5.50	107.77	114.92
1	A	255	GLY	N-CA-C	-5.49	107.78	114.92
1	A	968	ASP	N-CA-C	5.48	116.85	108.30
1	B	968	ASP	N-CA-C	5.47	116.83	108.30
1	A	713	GLU	N-CA-C	-5.46	105.75	112.90
1	A	27	ILE	N-CA-CB	-5.44	104.91	112.52
1	B	713	GLU	N-CA-C	-5.44	105.78	112.90
1	A	1023	LYS	N-CA-C	-5.43	101.81	109.96
1	B	1023	LYS	N-CA-C	-5.42	101.83	109.96
1	B	27	ILE	N-CA-CB	-5.42	104.93	112.52
1	A	771	ARG	N-CA-C	5.42	122.34	110.80
1	B	774	GLN	N-CA-C	5.41	119.73	113.18
1	B	771	ARG	N-CA-C	5.41	122.32	110.80
1	B	571	ALA	N-CA-C	5.40	117.92	111.71
1	A	774	GLN	N-CA-C	5.39	119.70	113.18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	GLU	N-CA-C	5.38	116.96	111.14
1	A	571	ALA	N-CA-C	5.38	117.89	111.71
1	B	535	ALA	N-CA-C	5.37	119.37	111.04
1	A	596	GLU	N-CA-C	5.37	116.94	111.14
1	A	535	ALA	N-CA-C	5.35	119.33	111.04
1	B	445	THR	N-CA-C	-5.34	101.00	108.96
1	A	725	GLU	N-CA-C	-5.33	101.85	110.32
1	A	445	THR	N-CA-C	-5.33	101.03	108.96
1	B	725	GLU	N-CA-C	-5.32	101.86	110.32
1	A	41	ASP	N-CA-C	5.29	118.20	111.69
1	B	1225	ASP	N-CA-C	-5.29	105.63	111.71
1	A	266	ALA	N-CA-C	5.28	116.54	109.83
1	A	1225	ASP	N-CA-C	-5.28	105.64	111.71
1	B	41	ASP	N-CA-C	5.28	118.18	111.69
1	B	266	ALA	N-CA-C	5.26	116.52	109.83
1	B	864	TRP	N-CA-C	5.26	118.06	109.59
1	A	864	TRP	N-CA-C	5.26	118.06	109.59
1	A	710	LYS	N-CA-C	-5.26	102.50	110.28
1	B	710	LYS	N-CA-C	-5.25	102.50	110.28
1	B	428	ASP	N-CA-C	-5.23	106.30	113.30
1	A	726	ALA	N-CA-C	5.22	117.24	109.25
1	A	428	ASP	N-CA-C	-5.22	106.31	113.30
1	B	726	ALA	N-CA-C	5.22	117.23	109.25
1	A	1171	ILE	CB-CA-C	-5.21	104.44	111.63
1	A	1173	GLU	N-CA-C	5.19	116.76	108.41
1	A	595	GLY	N-CA-C	5.18	125.47	113.18
1	B	595	GLY	N-CA-C	5.18	125.45	113.18
1	B	1173	GLU	N-CA-C	5.18	116.75	108.41
1	B	1141	PHE	CA-C-N	5.18	124.63	119.24
1	B	1141	PHE	C-N-CA	5.18	124.63	119.24
1	B	1171	ILE	CB-CA-C	-5.18	104.48	111.63
1	A	427	ALA	N-CA-C	5.17	118.85	112.24
1	B	427	ALA	N-CA-C	5.14	118.82	112.24
1	A	1141	PHE	CA-C-N	5.12	124.57	119.24
1	A	1141	PHE	C-N-CA	5.12	124.57	119.24
1	A	254	THR	N-CA-C	5.11	119.51	113.12
1	B	254	THR	N-CA-C	5.11	119.51	113.12
1	A	80	LEU	N-CA-C	-5.10	102.14	110.20
1	B	1167	ALA	N-CA-C	-5.09	105.73	111.28
1	A	616	PHE	N-CA-C	-5.09	101.47	109.25
1	B	80	LEU	N-CA-C	-5.09	102.16	110.20
1	B	155	VAL	CB-CA-C	-5.08	105.37	111.88

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	VAL	CB-CA-C	-5.08	105.38	111.88
1	A	693	ASN	N-CA-C	5.07	118.77	112.58
1	A	677	VAL	N-CA-C	5.07	117.77	112.90
1	B	693	ASN	N-CA-C	5.07	118.76	112.58
1	B	76	ALA	N-CA-C	-5.07	105.03	111.11
1	A	1167	ALA	N-CA-C	-5.06	105.76	111.28
1	B	616	PHE	N-CA-C	-5.05	101.53	109.25
1	B	677	VAL	N-CA-C	5.04	117.74	112.90
1	A	76	ALA	N-CA-C	-5.04	105.07	111.11
1	A	82	THR	CB-CA-C	-5.03	99.45	110.67
1	B	82	THR	CB-CA-C	-5.03	99.45	110.67
1	A	836	ASN	N-CA-C	5.03	116.95	108.96
1	B	836	ASN	N-CA-C	5.02	116.94	108.96
1	A	769	THR	N-CA-C	-5.01	107.17	113.28
1	A	278	SER	N-CA-C	5.00	119.02	113.01
1	B	594	LYS	N-CA-C	-5.00	99.63	108.23

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9382	0	9263	486	4
1	B	9382	0	9263	489	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	0	4	0
4	B	24	0	0	4	0
5	A	26	0	16	6	0
5	B	26	0	16	6	0
6	A	6	0	0	2	0
6	B	6	0	0	2	0
7	A	7	0	0	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	7	0	0	0	0
All	All	18894	0	18558	922	4

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 25.

All (922) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:GLY:HA3	1:B:1141:PHE:HZ	1.17	1.08
1:B:805:LEU:HA	1:B:854:LYS:HZ2	1.17	1.06
1:A:805:LEU:HA	1:A:854:LYS:HZ2	1.20	1.05
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.37	1.04
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.37	1.02
1:A:68:ALA:HB2	1:A:93:MET:HG2	1.46	0.97
1:B:68:ALA:HB2	1:B:93:MET:HG2	1.46	0.97
1:A:1141:PHE:HZ	1:B:1184:GLY:HA3	1.31	0.95
1:A:1184:GLY:HA3	1:B:1141:PHE:CZ	2.02	0.94
1:A:805:LEU:HA	1:A:854:LYS:NZ	1.83	0.92
1:B:805:LEU:HA	1:B:854:LYS:NZ	1.83	0.92
1:B:1149:ARG:HG3	1:B:1149:ARG:HH11	1.36	0.91
1:A:1149:ARG:HG3	1:A:1149:ARG:HH11	1.36	0.90
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.75	0.86
1:B:1132:ASN:O	1:B:1136:VAL:HG22	1.75	0.86
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.58	0.85
1:B:832:MET:HE2	1:B:834:ILE:HD11	1.58	0.85
1:A:832:MET:HE2	1:A:834:ILE:HD11	1.58	0.85
1:B:554:GLY:HA3	1:B:601:MET:HE2	1.58	0.85
1:A:9:ASP:OD1	1:A:12:THR:HG23	1.77	0.84
1:B:9:ASP:OD1	1:B:12:THR:HG23	1.77	0.84
1:A:492:PRO:O	1:A:495:VAL:HG12	1.78	0.84
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.60	0.83
1:A:554:GLY:HA3	1:A:601:MET:HE2	1.58	0.83
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.58	0.83
1:B:110:HIS:CD2	1:B:169:HIS:HD2	1.97	0.82
1:B:1000:GLN:HA	1:B:1012:LYS:HB2	1.60	0.82
1:B:99:LYS:O	1:B:103:GLU:HG3	1.79	0.82
1:B:492:PRO:O	1:B:495:VAL:HG12	1.78	0.82
1:A:110:HIS:CD2	1:A:169:HIS:HD2	1.97	0.81
1:B:349:VAL:HA	1:B:355:MET:HE1	1.62	0.81
1:A:99:LYS:O	1:A:103:GLU:HG3	1.79	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HG13	1:A:131:TYR:N	1.95	0.80
1:A:349:VAL:HA	1:A:355:MET:HE1	1.62	0.80
1:A:688:ASN:ND2	1:A:759:GLU:HB2	1.97	0.80
1:B:831:ARG:HD2	1:B:954:LYS:O	1.82	0.80
1:A:1184:GLY:CA	1:B:1141:PHE:HZ	1.95	0.80
1:B:544:ILE:HD12	1:B:613:LEU:HD13	1.63	0.80
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.63	0.80
1:B:130:ILE:HG13	1:B:131:TYR:N	1.95	0.79
1:A:831:ARG:HD2	1:A:954:LYS:O	1.82	0.79
1:A:544:ILE:HD12	1:A:613:LEU:HD13	1.63	0.79
1:B:688:ASN:ND2	1:B:759:GLU:HB2	1.97	0.78
1:A:755:CYS:SG	1:A:761:ALA:HB3	2.23	0.78
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.23	0.77
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.32	0.77
1:A:1141:PHE:CZ	1:B:1184:GLY:HA3	2.18	0.77
1:A:330:THR:O	1:A:362:ARG:HD3	1.84	0.77
1:A:1132:ASN:HD21	1:A:1139:ARG:HH12	1.32	0.77
1:B:739:GLN:HE22	1:B:777:ASN:HB3	1.50	0.77
1:B:330:THR:O	1:B:362:ARG:HD3	1.84	0.77
1:B:697:PHE:CE1	1:B:1042:MET:HE2	2.20	0.77
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.49	0.76
1:A:697:PHE:CE1	1:A:1042:MET:HE2	2.20	0.76
5:B:1243:TPP:H7'2	6:B:1246:PYR:O	1.86	0.76
1:A:1193:GLU:OE1	1:B:1077:ARG:HA	1.86	0.76
1:B:1137:LEU:HD22	1:B:1141:PHE:HB2	1.67	0.76
1:A:639:PHE:CE2	1:A:672:PHE:HB2	2.22	0.75
1:A:1137:LEU:HD22	1:A:1141:PHE:HB2	1.67	0.75
5:A:1236:TPP:H7'2	6:A:1239:PYR:O	1.86	0.75
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.36	0.74
1:B:639:PHE:CE2	1:B:672:PHE:HB2	2.22	0.74
1:A:857:ARG:HG3	1:A:858:LEU:HD13	1.69	0.74
1:A:24:VAL:HG13	1:B:881:MET:HE2	1.69	0.74
1:B:857:ARG:HG3	1:B:858:LEU:HD13	1.69	0.74
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.36	0.74
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.69	0.73
1:A:234:PRO:HA	1:A:237:LEU:HD12	1.71	0.73
1:A:1200:THR:HG23	1:A:1202:MET:HE3	1.72	0.72
1:B:234:PRO:HA	1:B:237:LEU:HD12	1.71	0.72
1:B:523:ASP:HA	1:B:531:LYS:NZ	2.05	0.72
1:B:1200:THR:HG23	1:B:1202:MET:HE3	1.72	0.72
1:B:14:THR:HG22	1:B:149:ALA:HB1	1.72	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.72	0.72
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.05	0.72
1:B:126:ASP:HA	1:B:329:ARG:HD3	1.71	0.71
1:A:126:ASP:HA	1:A:329:ARG:HD3	1.71	0.71
1:A:523:ASP:HA	1:A:531:LYS:HZ3	1.56	0.70
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.71	0.70
1:A:561:MET:HE1	1:A:583:LEU:HD21	1.71	0.70
1:B:180:ILE:HD11	1:B:438:ILE:HG21	1.72	0.70
1:A:130:ILE:HG13	1:A:131:TYR:H	1.56	0.70
1:B:82:THR:HG22	1:B:83:THR:H	1.57	0.69
1:A:180:ILE:HD11	1:A:438:ILE:HG21	1.72	0.69
1:A:467:HIS:HB3	1:A:481:VAL:HG23	1.75	0.69
1:A:873:ALA:HA	1:A:959:ILE:HD13	1.75	0.68
1:B:130:ILE:HG13	1:B:131:TYR:H	1.56	0.68
1:A:697:PHE:HD2	1:A:800:GLN:NE2	1.92	0.68
1:B:467:HIS:HB3	1:B:481:VAL:HG23	1.75	0.68
1:B:643:VAL:O	1:B:647:LEU:HG	1.94	0.68
1:A:82:THR:HG22	1:A:83:THR:H	1.57	0.67
1:A:643:VAL:O	1:A:647:LEU:HG	1.94	0.67
1:B:883:MET:O	1:B:887:ARG:HB2	1.95	0.67
1:B:1129:MET:HE3	1:B:1149:ARG:NE	2.09	0.67
1:A:883:MET:O	1:A:887:ARG:HB2	1.95	0.67
1:A:1129:MET:HE3	1:A:1149:ARG:NE	2.09	0.67
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.75	0.67
1:B:697:PHE:HD2	1:B:800:GLN:NE2	1.92	0.66
1:A:1181:LYS:H	1:B:1019:ARG:HH12	1.43	0.66
1:A:460:SER:HB3	1:A:746:MET:HE2	1.77	0.66
1:A:1166:MET:O	1:A:1169:THR:HG22	1.96	0.66
1:A:141:LEU:HD13	1:A:152:MET:HG3	1.77	0.66
1:B:1077:ARG:HH11	1:B:1077:ARG:HB2	1.61	0.66
1:B:771:ARG:O	1:B:775:VAL:HG23	1.96	0.66
1:B:460:SER:HB3	1:B:746:MET:HE2	1.77	0.65
1:A:771:ARG:O	1:A:775:VAL:HG23	1.96	0.65
1:B:1035:VAL:HG22	1:B:1062:PRO:HB2	1.79	0.65
1:B:1166:MET:O	1:B:1169:THR:HG22	1.96	0.65
1:A:456:ASP:HB2	1:A:463:ILE:O	1.96	0.65
1:A:881:MET:HE2	1:B:24:VAL:HG13	1.79	0.65
1:B:141:LEU:HD13	1:B:152:MET:HG3	1.77	0.65
1:A:1077:ARG:HH11	1:A:1077:ARG:HB2	1.61	0.64
1:A:154:LEU:HD22	1:A:158:LEU:HD11	1.79	0.64
1:B:456:ASP:HB2	1:B:463:ILE:O	1.96	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:LEU:HB3	1:A:853:TYR:O	1.97	0.64
1:B:154:LEU:HD22	1:B:158:LEU:HD11	1.80	0.64
1:A:1035:VAL:HG22	1:A:1062:PRO:HB2	1.79	0.64
1:B:667:LEU:HB3	1:B:853:TYR:O	1.97	0.64
1:B:697:PHE:HE1	1:B:1042:MET:HE2	1.62	0.64
1:A:368:LYS:NZ	1:B:227:GLN:HE22	1.95	0.64
1:A:1216:ARG:HA	1:B:746:MET:O	1.97	0.64
1:B:968:ASP:OD1	1:B:1003:LYS:HB2	1.99	0.63
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.14	0.63
1:A:730:GLU:CD	1:A:730:GLU:H	2.05	0.63
1:A:779:GLU:HB3	1:A:783:ARG:NH1	2.13	0.63
1:B:64:GLU:HG3	1:B:89:GLY:HA2	1.81	0.63
1:B:730:GLU:H	1:B:730:GLU:CD	2.05	0.63
1:B:1193:GLU:N	1:B:1193:GLU:CD	2.57	0.63
1:B:523:ASP:HA	1:B:531:LYS:HZ3	1.63	0.63
1:B:779:GLU:HB3	1:B:783:ARG:NH1	2.13	0.63
1:A:64:GLU:HG3	1:A:89:GLY:HA2	1.81	0.63
1:B:445:THR:HG21	1:B:574:LEU:HD21	1.80	0.63
1:B:1200:THR:CG2	1:B:1202:MET:HE3	2.29	0.63
1:A:34:SER:O	1:A:38:GLU:HG3	1.98	0.63
1:A:917:LYS:HB3	1:A:917:LYS:HZ3	1.64	0.63
1:B:34:SER:O	1:B:38:GLU:HG3	1.97	0.63
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.80	0.62
1:B:438:ILE:HG23	1:B:449:ALA:HB1	1.80	0.62
1:B:890:LEU:HD11	1:B:945:ILE:HG23	1.81	0.62
1:A:1193:GLU:CD	1:A:1193:GLU:N	2.57	0.62
1:B:1198:ASP:OD1	1:B:1200:THR:HB	2.00	0.62
1:A:890:LEU:HD11	1:A:945:ILE:HG23	1.81	0.62
1:A:968:ASP:OD1	1:A:1003:LYS:HB2	1.99	0.62
1:A:438:ILE:HG23	1:A:449:ALA:HB1	1.80	0.62
1:A:1141:PHE:HZ	1:B:1184:GLY:CA	2.10	0.62
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.14	0.62
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.35	0.62
1:A:325:THR:CG2	1:A:382:MET:SD	2.88	0.62
1:B:522:MET:SD	1:B:526:LEU:HD13	2.40	0.62
1:A:1200:THR:CG2	1:A:1202:MET:HE3	2.29	0.62
1:B:142:ALA:HB2	1:B:170:PHE:CZ	2.35	0.62
1:A:1198:ASP:OD1	1:A:1200:THR:HB	1.99	0.62
1:B:467:HIS:CD2	1:B:481:VAL:H	2.18	0.61
1:A:325:THR:HG23	1:A:382:MET:SD	2.40	0.61
1:B:325:THR:CG2	1:B:382:MET:SD	2.88	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:HIS:CD2	1:A:481:VAL:H	2.18	0.61
1:B:148:GLU:O	1:B:152:MET:HB2	2.00	0.61
1:A:148:GLU:O	1:A:152:MET:HB2	2.00	0.61
1:B:325:THR:HG23	1:B:382:MET:SD	2.41	0.61
1:B:1124:VAL:O	1:B:1127:PHE:HB3	2.01	0.61
1:A:398:VAL:HG13	1:A:656:VAL:CG2	2.31	0.61
1:A:180:ILE:HD11	1:A:438:ILE:CG2	2.30	0.61
1:A:522:MET:SD	1:A:526:LEU:HD13	2.40	0.61
1:A:1124:VAL:O	1:A:1127:PHE:HB3	2.01	0.61
1:B:180:ILE:HD11	1:B:438:ILE:CG2	2.30	0.60
1:B:398:VAL:HG13	1:B:656:VAL:CG2	2.31	0.60
1:A:993:VAL:HG22	1:A:1000:GLN:O	2.01	0.60
1:A:697:PHE:HE1	1:A:1042:MET:HE2	1.62	0.60
1:A:154:LEU:HD22	1:A:158:LEU:CD1	2.31	0.60
1:A:465:ILE:HD12	1:A:466:SER:N	2.17	0.60
1:B:1129:MET:HE3	1:B:1149:ARG:CZ	2.31	0.60
1:B:993:VAL:HG22	1:B:1000:GLN:O	2.01	0.60
1:B:917:LYS:HZ3	1:B:917:LYS:HB3	1.66	0.59
1:B:779:GLU:HB3	1:B:783:ARG:HH12	1.68	0.59
1:A:976:HIS:CD2	1:B:1003:LYS:HD3	2.38	0.59
1:A:1129:MET:HE3	1:A:1149:ARG:CZ	2.32	0.59
1:B:1193:GLU:CD	1:B:1193:GLU:H	2.11	0.59
1:B:154:LEU:HD22	1:B:158:LEU:CD1	2.31	0.59
1:A:236:TYR:HA	1:A:239:VAL:HG12	1.84	0.59
1:B:465:ILE:HD12	1:B:466:SER:N	2.17	0.59
1:A:700:PRO:HG3	1:A:814:GLY:HA2	1.85	0.59
1:A:1016:ALA:HB1	1:A:1019:ARG:HH21	1.66	0.59
1:A:549:ILE:O	1:A:553:VAL:HG22	2.03	0.59
1:B:700:PRO:HG3	1:B:814:GLY:HA2	1.85	0.59
1:A:356:PRO:O	1:A:357:LYS:HB3	2.02	0.59
1:A:1181:LYS:H	1:B:1019:ARG:NH1	2.01	0.59
1:B:549:ILE:O	1:B:553:VAL:HG22	2.03	0.59
1:B:639:PHE:CD2	1:B:672:PHE:HB2	2.37	0.59
1:B:894:ALA:CB	1:B:914:LEU:HD21	2.33	0.59
1:B:917:LYS:HB3	1:B:917:LYS:NZ	2.18	0.59
1:A:87:SER:HA	1:A:129:ASP:HB3	1.85	0.59
1:A:639:PHE:CD2	1:A:672:PHE:HB2	2.37	0.59
1:A:676:GLY:HA3	1:A:743:LEU:HD22	1.84	0.59
1:A:917:LYS:HB3	1:A:917:LYS:NZ	2.18	0.59
1:A:494:TYR:HB3	1:A:500:ILE:HD11	1.84	0.59
1:A:894:ALA:CB	1:A:914:LEU:HD21	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:GLN:HE21	1:A:1048:GLN:C	2.11	0.58
1:A:1077:ARG:HA	1:B:1193:GLU:OE1	2.02	0.58
1:B:494:TYR:HB3	1:B:500:ILE:HD11	1.84	0.58
1:A:396:ASP:HA	1:A:656:VAL:HG13	1.84	0.58
1:A:832:MET:HE2	1:A:834:ILE:CD1	2.31	0.58
1:B:87:SER:HA	1:B:129:ASP:HB3	1.85	0.58
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.85	0.58
1:B:676:GLY:HA3	1:B:743:LEU:HD22	1.84	0.58
1:A:9:ASP:HA	1:A:179:GLU:O	2.03	0.58
1:A:460:SER:HB3	1:A:746:MET:CE	2.33	0.58
1:A:643:VAL:HB	1:A:849:PRO:HB2	1.85	0.58
1:B:894:ALA:HB3	1:B:914:LEU:HD21	1.86	0.58
1:B:1016:ALA:HB1	1:B:1019:ARG:HH21	1.66	0.58
1:A:263:TYR:CZ	1:A:318:PRO:HG2	2.38	0.58
1:A:699:CYS:SG	1:A:703:ALA:HB3	2.44	0.58
1:A:1193:GLU:CD	1:A:1193:GLU:H	2.11	0.58
1:B:396:ASP:HA	1:B:656:VAL:HG13	1.84	0.58
1:B:806:MET:SD	1:B:852:PRO:HB2	2.44	0.58
1:B:1048:GLN:C	1:B:1048:GLN:HE21	2.11	0.58
1:A:779:GLU:HB3	1:A:783:ARG:HH12	1.68	0.58
1:A:894:ALA:HB3	1:A:914:LEU:HD21	1.86	0.58
1:B:699:CYS:SG	1:B:703:ALA:HB3	2.44	0.58
1:B:10:GLY:O	1:B:14:THR:HG23	2.04	0.58
1:A:806:MET:SD	1:A:852:PRO:HB2	2.44	0.58
1:A:1160:PHE:O	1:A:1164:GLU:HG3	2.04	0.57
1:B:4:LYS:HB3	1:B:185:VAL:HG23	1.86	0.57
1:B:236:TYR:HA	1:B:239:VAL:HG12	1.84	0.57
1:A:10:GLY:O	1:A:14:THR:HG23	2.04	0.57
1:B:460:SER:HB3	1:B:746:MET:CE	2.33	0.57
1:B:9:ASP:HA	1:B:179:GLU:O	2.03	0.57
1:B:356:PRO:O	1:B:357:LYS:HB3	2.02	0.57
1:B:1160:PHE:O	1:B:1164:GLU:HG3	2.04	0.57
1:A:4:LYS:HB3	1:A:185:VAL:HG23	1.86	0.57
1:B:20:ALA:HB2	1:B:188:TYR:CE1	2.39	0.57
1:B:263:TYR:CZ	1:B:318:PRO:HG2	2.38	0.57
1:A:20:ALA:HB2	1:A:188:TYR:CE1	2.39	0.57
1:A:565:THR:HG21	1:A:609:ALA:HB3	1.87	0.57
1:A:1219:THR:CG2	1:A:1221:GLU:HG2	2.35	0.57
5:B:1243:TPP:H2	5:B:1243:TPP:HN42	1.70	0.57
1:B:495:VAL:HG23	1:B:530:ILE:HD12	1.87	0.57
1:A:697:PHE:CD2	1:A:800:GLN:NE2	2.73	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:ASP:CG	1:A:1104:ARG:HH11	2.14	0.56
1:B:1219:THR:CG2	1:B:1221:GLU:HG2	2.35	0.56
1:A:1219:THR:HG21	1:B:1082:LYS:HZ3	1.70	0.56
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.22	0.56
1:A:986:VAL:HG22	1:A:1064:LEU:HD23	1.88	0.56
1:B:345:CYS:O	1:B:349:VAL:HG13	2.06	0.56
1:A:1215:ASN:ND2	1:B:1080:MET:H	2.03	0.56
1:B:467:HIS:HD2	1:B:481:VAL:H	1.53	0.56
1:B:697:PHE:CD2	1:B:800:GLN:NE2	2.73	0.56
1:B:986:VAL:HG22	1:B:1064:LEU:HD23	1.88	0.56
1:B:1225:ASP:O	1:B:1229:ARG:HG3	2.06	0.56
1:B:434:ASN:O	1:B:438:ILE:HG13	2.06	0.56
1:B:565:THR:HG21	1:B:609:ALA:HB3	1.87	0.56
1:B:832:MET:HE2	1:B:834:ILE:CD1	2.31	0.56
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.40	0.56
1:B:124:PHE:CB	1:B:367:SER:HB2	2.26	0.55
1:B:1004:ALA:O	1:B:1022:LYS:HG3	2.06	0.55
1:B:1102:ASP:CG	1:B:1104:ARG:HH11	2.14	0.55
5:A:1236:TPP:H2	5:A:1236:TPP:HN42	1.70	0.55
1:B:290:LEU:HG	1:B:295:GLU:OE1	2.07	0.55
1:A:1004:ALA:O	1:A:1022:LYS:HG3	2.06	0.55
1:A:1225:ASP:O	1:A:1229:ARG:HG3	2.06	0.55
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.40	0.55
1:A:345:CYS:O	1:A:349:VAL:HG13	2.06	0.55
1:B:681:VAL:HG23	1:B:770:GLN:HG3	1.88	0.55
1:B:715:VAL:C	1:B:717:ALA:H	2.14	0.55
1:A:561:MET:HE1	1:A:583:LEU:CD2	2.36	0.55
1:A:495:VAL:HG23	1:A:530:ILE:HD12	1.87	0.55
1:A:563:MET:HE3	1:A:563:MET:HA	1.89	0.55
1:B:260:LEU:O	1:B:303:ARG:HB2	2.07	0.55
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.72	0.55
5:B:1243:TPP:H7'2	6:B:1246:PYR:C	2.36	0.55
1:A:536:ASN:HD22	1:A:623:LYS:NZ	2.05	0.55
5:A:1236:TPP:H7'2	6:A:1239:PYR:C	2.36	0.55
1:B:331:LYS:HG3	1:B:331:LYS:O	2.06	0.55
1:A:681:VAL:HG23	1:A:770:GLN:HG3	1.88	0.55
1:B:1219:THR:HG22	1:B:1222:GLN:H	1.72	0.55
1:A:434:ASN:O	1:A:438:ILE:HG13	2.06	0.55
1:B:495:VAL:HG13	1:B:496:GLY:N	2.22	0.55
1:A:456:ASP:OD1	1:A:458:LYS:HB2	2.07	0.55
1:B:110:HIS:CD2	1:B:169:HIS:CD2	2.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1077:ARG:HB2	1:B:1077:ARG:NH1	2.22	0.55
1:B:422:PHE:HE1	1:B:468:LEU:HG	1.72	0.54
1:A:422:PHE:HE1	1:A:468:LEU:HG	1.72	0.54
1:A:495:VAL:HG13	1:A:496:GLY:N	2.22	0.54
1:A:715:VAL:C	1:A:717:ALA:H	2.13	0.54
1:B:563:MET:HE3	1:B:563:MET:HA	1.89	0.54
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.72	0.54
1:B:58:ILE:HD12	1:B:58:ILE:H	1.72	0.54
1:B:456:ASP:OD1	1:B:458:LYS:HB2	2.07	0.54
1:B:561:MET:HE1	1:B:583:LEU:CD2	2.36	0.54
1:B:1146:LYS:HA	1:B:1149:ARG:HH12	1.72	0.54
1:A:495:VAL:HG13	1:A:496:GLY:H	1.73	0.54
1:A:260:LEU:O	1:A:303:ARG:HB2	2.07	0.54
1:A:434:ASN:HD22	1:A:453:PHE:HE1	1.56	0.54
1:A:467:HIS:HD2	1:A:481:VAL:H	1.54	0.54
1:A:99:LYS:HE3	1:B:867:SER:O	2.06	0.54
1:A:249:LYS:O	1:A:252:SER:HB3	2.07	0.54
1:A:1146:LYS:HA	1:A:1149:ARG:HH12	1.72	0.54
1:B:323:VAL:CG1	1:B:382:MET:HG2	2.38	0.54
1:B:688:ASN:HD21	1:B:759:GLU:HB2	1.73	0.54
1:B:1149:ARG:HH11	1:B:1149:ARG:CG	2.16	0.54
1:A:64:GLU:HB2	1:A:93:MET:HE3	1.89	0.54
1:A:210:PRO:HB2	1:B:831:ARG:HA	1.89	0.54
1:A:290:LEU:HG	1:A:295:GLU:OE1	2.07	0.54
1:A:1131:GLN:OE1	1:A:1133:ARG:NE	2.40	0.54
1:A:497:ILE:HG13	1:A:498:TYR:CD2	2.43	0.53
1:B:536:ASN:HD22	1:B:623:LYS:NZ	2.05	0.53
1:B:817:GLU:HB3	1:B:989:MET:HE3	1.90	0.53
1:A:227:GLN:HE22	1:B:368:LYS:NZ	2.07	0.53
1:A:609:ALA:O	1:A:613:LEU:HB2	2.08	0.53
1:B:249:LYS:O	1:B:252:SER:HB3	2.07	0.53
1:B:1230:THR:O	1:B:1232:LYS:N	2.42	0.53
1:A:323:VAL:CG1	1:A:382:MET:HG2	2.38	0.53
1:A:688:ASN:HD21	1:A:759:GLU:HB2	1.73	0.53
1:A:1194:PHE:CD2	1:A:1213:ASP:HB3	2.44	0.53
1:B:495:VAL:HG13	1:B:496:GLY:H	1.73	0.53
1:A:1219:THR:HG21	1:B:1082:LYS:NZ	2.24	0.53
1:A:331:LYS:O	1:A:331:LYS:HG3	2.06	0.53
1:A:536:ASN:HD22	1:A:623:LYS:HZ3	1.57	0.53
1:A:699:CYS:HA	4:A:1234:SF4:S2	2.48	0.53
1:A:1080:MET:O	1:A:1083:SER:HB2	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:MET:O	1:B:1083:SER:HB2	2.08	0.53
1:A:110:HIS:CD2	1:A:169:HIS:CD2	2.88	0.53
1:A:817:GLU:HB3	1:A:989:MET:HE3	1.91	0.53
1:B:609:ALA:O	1:B:613:LEU:HB2	2.08	0.53
1:A:463:ILE:HG13	1:A:464:THR:N	2.24	0.53
1:A:903:SER:O	1:A:907:LYS:HG3	2.08	0.53
1:B:64:GLU:HB2	1:B:93:MET:HE3	1.89	0.53
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.39	0.53
1:B:867:SER:O	1:B:868:LEU:HD23	2.09	0.53
1:B:903:SER:O	1:B:907:LYS:HG3	2.08	0.53
1:B:1131:GLN:OE1	1:B:1133:ARG:NE	2.40	0.53
1:A:1077:ARG:HB2	1:A:1077:ARG:NH1	2.22	0.53
1:B:630:LYS:HD2	1:B:632:GLU:HG2	1.91	0.53
1:B:1194:PHE:CD2	1:B:1213:ASP:HB3	2.44	0.53
1:A:630:LYS:HD2	1:A:632:GLU:HG2	1.91	0.53
1:A:1149:ARG:HH11	1:A:1149:ARG:CG	2.16	0.53
1:A:398:VAL:HG13	1:A:656:VAL:HG22	1.91	0.52
1:A:1059:PHE:HD1	1:A:1104:ARG:HD3	1.75	0.52
1:A:1082:LYS:HZ3	1:B:1219:THR:HG21	1.74	0.52
1:B:534:ILE:HA	1:B:539:LEU:HG	1.91	0.52
1:B:619:PRO:HG2	1:B:622:TRP:CD1	2.44	0.52
1:A:867:SER:O	1:A:868:LEU:HD23	2.09	0.52
1:A:1230:THR:O	1:A:1232:LYS:N	2.42	0.52
1:B:497:ILE:HG13	1:B:498:TYR:CD2	2.43	0.52
1:B:699:CYS:HA	4:B:1241:SF4:S2	2.48	0.52
1:A:81:THR:HG22	1:A:82:THR:N	2.24	0.52
1:A:387:LYS:HD3	1:A:390:PHE:HB3	1.91	0.52
1:A:1019:ARG:HH12	1:B:1181:LYS:H	1.57	0.52
1:B:434:ASN:HD22	1:B:453:PHE:HE1	1.56	0.52
1:A:964:GLY:O	1:A:968:ASP:HB2	2.10	0.52
1:A:323:VAL:HA	1:A:356:PRO:O	2.09	0.52
1:B:387:LYS:HD3	1:B:390:PHE:HB3	1.91	0.52
1:B:775:VAL:HB	1:B:776:PRO:CD	2.40	0.52
1:B:964:GLY:O	1:B:968:ASP:HB2	2.10	0.52
1:A:775:VAL:HB	1:A:776:PRO:CD	2.40	0.52
1:B:398:VAL:HG13	1:B:656:VAL:HG22	1.91	0.52
1:A:58:ILE:HD12	1:A:58:ILE:H	1.72	0.52
1:B:463:ILE:HG13	1:B:464:THR:N	2.24	0.52
1:B:1059:PHE:HD1	1:B:1104:ARG:HD3	1.75	0.52
1:A:230:GLU:OE2	1:B:331:LYS:HE3	2.09	0.52
1:A:534:ILE:HA	1:A:539:LEU:HG	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:TYR:O	1:B:1063:SER:HA	2.10	0.52
1:A:619:PRO:HG2	1:A:622:TRP:CD1	2.44	0.52
1:A:853:TYR:CE2	1:A:864:TRP:CD1	2.98	0.52
1:A:1035:VAL:O	1:A:1037:VAL:HG23	2.10	0.52
1:B:323:VAL:HA	1:B:356:PRO:O	2.09	0.52
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.39	0.51
1:A:681:VAL:HG22	1:A:767:LEU:HA	1.91	0.51
1:B:81:THR:HG22	1:B:82:THR:N	2.24	0.51
1:A:269:ALA:HA	1:A:296:LYS:HB3	1.92	0.51
1:A:873:ALA:HA	1:A:959:ILE:HG21	1.92	0.51
1:A:961:GLY:O	1:A:988:VAL:HA	2.11	0.51
1:A:1025:LEU:O	1:A:1029:VAL:HG13	2.11	0.51
1:A:1036:TYR:O	1:A:1063:SER:HA	2.10	0.51
1:B:873:ALA:HA	1:B:959:ILE:HG21	1.92	0.51
1:A:105:LEU:O	1:A:166:PRO:HG3	2.11	0.51
1:A:695:CYS:HB2	1:A:704:ILE:HD13	1.92	0.51
1:B:349:VAL:CG2	1:B:350:GLU:N	2.73	0.51
1:B:853:TYR:CE2	1:B:864:TRP:CD1	2.98	0.51
1:A:1138:ASP:O	1:A:1142:PRO:HG3	2.10	0.51
1:B:465:ILE:HG13	1:B:467:HIS:CE1	2.46	0.51
1:A:465:ILE:HG13	1:A:467:HIS:CE1	2.46	0.51
1:B:105:LEU:O	1:B:166:PRO:HG3	2.11	0.51
1:A:349:VAL:CG2	1:A:350:GLU:N	2.73	0.51
1:B:1016:ALA:HB1	1:B:1019:ARG:NH2	2.26	0.51
1:B:1035:VAL:O	1:B:1037:VAL:HG23	2.10	0.51
1:A:715:VAL:HG12	1:A:716:GLY:N	2.25	0.51
1:A:1160:PHE:O	1:A:1160:PHE:CD1	2.64	0.51
1:B:681:VAL:HG22	1:B:767:LEU:HA	1.91	0.51
1:B:695:CYS:HB2	1:B:704:ILE:HD13	1.92	0.51
1:B:1138:ASP:O	1:B:1142:PRO:HG3	2.10	0.51
1:B:715:VAL:HG12	1:B:716:GLY:N	2.25	0.50
1:B:1160:PHE:O	1:B:1160:PHE:CD1	2.64	0.50
1:B:1025:LEU:O	1:B:1029:VAL:HG13	2.11	0.50
1:A:130:ILE:HD13	1:A:170:PHE:CZ	2.46	0.50
1:A:910:LEU:HD12	1:A:930:LEU:HD21	1.92	0.50
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.22	0.50
1:B:131:TYR:O	1:B:134:ARG:HB2	2.12	0.50
1:B:902:ALA:O	1:B:907:LYS:HE3	2.11	0.50
1:A:491:ASN:C	1:A:491:ASN:HD22	2.19	0.50
1:B:691:GLN:HG2	1:B:736:PHE:CD1	2.47	0.50
1:B:910:LEU:HD12	1:B:930:LEU:HD21	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:LEU:HD13	1:B:930:LEU:HD11	1.93	0.50
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.47	0.50
1:B:269:ALA:HA	1:B:296:LYS:HB3	1.92	0.50
1:A:82:THR:HG22	1:A:83:THR:N	2.27	0.50
1:A:131:TYR:O	1:A:134:ARG:HB2	2.12	0.50
1:A:684:TRP:CE2	1:A:738:ILE:HB	2.47	0.50
1:A:1016:ALA:HB1	1:A:1019:ARG:NH2	2.26	0.50
1:B:578:LYS:HE3	1:B:582:LEU:HD21	1.94	0.50
1:A:691:GLN:HG2	1:A:736:PHE:CD1	2.47	0.50
1:B:491:ASN:C	1:B:491:ASN:HD22	2.19	0.50
1:B:578:LYS:HG3	1:B:582:LEU:HD22	1.94	0.50
1:B:587:ILE:O	1:B:591:TYR:HB2	2.12	0.50
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.46	0.50
1:B:963:ASP:HB3	1:B:990:ASP:OD1	2.12	0.50
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.94	0.50
1:A:216:ARG:O	1:B:865:GLY:HA2	2.12	0.50
1:A:578:LYS:HE3	1:A:582:LEU:HD21	1.94	0.50
1:A:721:PHE:HD1	1:A:777:ASN:HD22	1.59	0.50
1:A:902:ALA:O	1:A:907:LYS:HE3	2.11	0.50
1:A:693:ASN:HB3	1:A:800:GLN:HB2	1.94	0.50
1:B:961:GLY:O	1:B:988:VAL:HA	2.11	0.50
1:B:130:ILE:HD13	1:B:170:PHE:CZ	2.46	0.49
1:B:200:LEU:HD11	1:B:204:ARG:NH1	2.27	0.49
1:A:200:LEU:HD11	1:A:204:ARG:NH1	2.27	0.49
1:A:553:VAL:O	1:A:601:MET:HG3	2.11	0.49
1:A:587:ILE:O	1:A:591:TYR:HB2	2.12	0.49
1:A:746:MET:O	1:B:1216:ARG:HA	2.12	0.49
1:A:910:LEU:HD13	1:A:930:LEU:HD11	1.93	0.49
1:B:182:LYS:HE2	1:B:442:GLY:O	2.13	0.49
1:A:323:VAL:HG12	1:A:382:MET:HG2	1.94	0.49
1:B:512:LEU:HD12	1:B:513:ASN:N	2.27	0.49
1:B:636:ASN:ND2	1:B:672:PHE:HE2	2.11	0.49
1:A:182:LYS:HE2	1:A:442:GLY:O	2.13	0.49
1:A:1188:PHE:HB3	1:B:1010:VAL:O	2.11	0.49
1:B:43:TRP:HB3	1:B:48:ARG:HD3	1.94	0.49
1:B:721:PHE:HD1	1:B:777:ASN:HD22	1.59	0.49
1:B:965:TRP:CE3	1:B:966:ALA:HB2	2.48	0.49
1:B:126:ASP:HA	1:B:329:ARG:CD	2.42	0.49
1:B:713:GLU:O	1:B:780:TYR:OH	2.31	0.49
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.78	0.49
1:A:264:VAL:HG21	1:A:301:LYS:HE3	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:MET:HE2	1:A:955:LYS:HD2	1.94	0.49
1:B:27:ILE:HG23	1:B:28:TYR:N	2.28	0.49
1:B:553:VAL:O	1:B:601:MET:HG3	2.11	0.49
1:A:334:GLY:O	1:B:307:PRO:HA	2.13	0.49
1:A:512:LEU:HD12	1:A:513:ASN:N	2.28	0.49
1:B:684:TRP:CE2	1:B:738:ILE:HB	2.47	0.49
1:A:965:TRP:CE3	1:A:966:ALA:HB2	2.48	0.49
1:B:323:VAL:HG12	1:B:382:MET:HG2	1.94	0.49
1:B:883:MET:HE2	1:B:955:LYS:HD2	1.94	0.49
1:A:992:GLU:O	1:A:993:VAL:HB	2.13	0.49
1:A:578:LYS:HG3	1:A:582:LEU:HD22	1.94	0.48
1:A:569:LYS:HB3	1:A:570:LEU:HD13	1.95	0.48
1:A:703:ALA:HB3	4:A:1234:SF4:S4	2.53	0.48
1:A:994:TYR:CE1	1:A:1002:SER:HB2	2.48	0.48
1:B:693:ASN:HB3	1:B:800:GLN:HB2	1.94	0.48
1:B:992:GLU:O	1:B:993:VAL:HB	2.13	0.48
1:A:27:ILE:HG23	1:A:28:TYR:N	2.28	0.48
1:A:681:VAL:CG2	1:A:767:LEU:HA	2.43	0.48
1:A:963:ASP:HB3	1:A:990:ASP:OD1	2.12	0.48
1:A:1129:MET:HE1	1:A:1138:ASP:HB2	1.95	0.48
1:B:23:GLU:OE1	1:B:204:ARG:NH2	2.46	0.48
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.78	0.48
1:B:703:ALA:HB3	4:B:1241:SF4:S4	2.53	0.48
1:A:60:GLU:O	1:B:976:HIS:HE1	1.96	0.48
1:A:583:LEU:O	1:A:587:ILE:HG12	2.13	0.48
1:A:834:ILE:HD13	1:A:960:PHE:CE2	2.49	0.48
1:A:940:GLY:O	1:A:943:GLY:N	2.46	0.48
1:B:264:VAL:HG21	1:B:301:LYS:HE3	1.93	0.48
1:B:590:ALA:O	1:B:591:TYR:HB2	2.14	0.48
1:A:23:GLU:OE1	1:A:204:ARG:NH2	2.46	0.48
1:A:274:VAL:HG23	1:A:324:ILE:CD1	2.44	0.48
1:A:1019:ARG:NH1	1:B:1181:LYS:H	2.12	0.48
1:B:226:PHE:HD1	1:B:226:PHE:O	1.96	0.48
1:B:42:ASP:O	1:B:46:GLN:HG3	2.14	0.48
1:B:684:TRP:CD2	1:B:738:ILE:HB	2.48	0.48
1:A:684:TRP:CD2	1:A:738:ILE:HB	2.48	0.48
1:A:42:ASP:O	1:A:46:GLN:HG3	2.14	0.48
1:A:338:ASP:OD2	1:A:362:ARG:NH1	2.47	0.48
1:A:681:VAL:HG12	1:A:745:CYS:SG	2.53	0.48
1:B:274:VAL:HG23	1:B:324:ILE:CD1	2.44	0.48
1:B:617:LYS:HB2	1:B:617:LYS:NZ	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:PHE:CE1	1:B:780:TYR:HD2	2.32	0.48
1:B:867:SER:HB2	1:B:875:TYR:CG	2.49	0.48
1:B:940:GLY:O	1:B:943:GLY:N	2.46	0.48
1:B:994:TYR:CE1	1:B:1002:SER:HB2	2.48	0.48
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.95	0.48
1:A:867:SER:HB2	1:A:875:TYR:CG	2.49	0.48
1:A:590:ALA:O	1:A:591:TYR:HB2	2.14	0.47
1:A:713:GLU:O	1:A:780:TYR:OH	2.31	0.47
1:A:736:PHE:CD1	1:A:736:PHE:C	2.92	0.47
1:B:736:PHE:CD1	1:B:736:PHE:C	2.92	0.47
1:B:799:SER:OG	1:B:800:GLN:NE2	2.47	0.47
1:A:1175:PHE:CZ	1:A:1177:PRO:HA	2.49	0.47
1:B:569:LYS:HB3	1:B:570:LEU:HD13	1.95	0.47
1:B:642:VAL:C	1:B:645:PRO:HD2	2.39	0.47
1:B:646:ILE:HG21	1:B:849:PRO:HD3	1.96	0.47
1:B:681:VAL:CG2	1:B:767:LEU:HA	2.43	0.47
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.14	0.47
1:A:154:LEU:HD13	1:A:250:VAL:HG22	1.96	0.47
1:A:795:SER:O	1:A:796:LEU:C	2.58	0.47
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.96	0.47
1:B:566:ALA:HA	1:B:613:LEU:HD21	1.95	0.47
1:B:871:ASP:HB2	1:B:874:GLU:HG2	1.96	0.47
1:B:1040:VAL:HA	1:B:1098:LEU:HD22	1.96	0.47
1:B:1129:MET:HE1	1:B:1138:ASP:HB2	1.95	0.47
1:B:146:VAL:HG12	1:B:183:ILE:HD13	1.96	0.47
1:A:636:ASN:ND2	1:A:672:PHE:HE2	2.11	0.47
1:A:710:LYS:HD2	1:A:734:TYR:HE1	1.80	0.47
1:A:799:SER:OG	1:A:800:GLN:NE2	2.47	0.47
1:B:681:VAL:HG12	1:B:745:CYS:SG	2.53	0.47
1:B:795:SER:O	1:B:796:LEU:C	2.58	0.47
1:A:146:VAL:HG12	1:A:183:ILE:HD13	1.96	0.47
1:A:226:PHE:HD1	1:A:226:PHE:O	1.96	0.47
1:A:286:VAL:HG12	1:A:290:LEU:HD22	1.97	0.47
1:B:121:LEU:HG	1:B:122:SER:N	2.29	0.47
1:B:338:ASP:OD2	1:B:362:ARG:NH1	2.47	0.47
1:B:536:ASN:HA	1:B:623:LYS:HZ3	1.79	0.47
1:B:583:LEU:O	1:B:587:ILE:HG12	2.13	0.47
1:B:710:LYS:HD2	1:B:734:TYR:HE1	1.80	0.47
1:B:814:GLY:O	1:B:1080:MET:HE3	2.15	0.47
1:B:834:ILE:HD13	1:B:960:PHE:CE2	2.49	0.47
1:A:617:LYS:HB2	1:A:617:LYS:NZ	2.28	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.14	0.47
1:A:1214:GLN:NE2	1:B:461:GLY:H	2.12	0.47
1:B:573:VAL:HG23	1:B:574:LEU:HG	1.97	0.47
1:B:1129:MET:HG2	1:B:1149:ARG:HE	1.80	0.47
1:B:1175:PHE:CZ	1:B:1177:PRO:HA	2.49	0.47
1:A:121:LEU:HG	1:A:122:SER:N	2.29	0.47
1:A:126:ASP:HA	1:A:329:ARG:CD	2.42	0.47
1:A:317:LEU:HD22	1:A:317:LEU:C	2.39	0.47
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.96	0.47
1:A:779:GLU:C	1:A:783:ARG:HH11	2.23	0.47
1:A:867:SER:O	1:B:99:LYS:HE3	2.15	0.47
1:A:871:ASP:HB2	1:A:874:GLU:HG2	1.96	0.47
1:B:64:GLU:HG3	1:B:89:GLY:CA	2.45	0.47
1:B:890:LEU:CD1	1:B:945:ILE:HG23	2.45	0.47
1:B:917:LYS:NZ	1:B:917:LYS:CB	2.78	0.47
1:A:14:THR:HG21	1:A:171:PHE:CE1	2.50	0.47
1:A:573:VAL:HG23	1:A:574:LEU:HG	1.97	0.47
1:A:646:ILE:HG21	1:A:849:PRO:HD3	1.96	0.47
1:A:1003:LYS:HD3	1:B:976:HIS:CD2	2.50	0.47
1:A:721:PHE:CE1	1:A:780:TYR:HD2	2.32	0.46
1:A:1214:GLN:CD	1:B:461:GLY:H	2.23	0.46
1:B:779:GLU:C	1:B:783:ARG:HH11	2.23	0.46
1:B:1007:THR:HB	1:B:1152:VAL:HG22	1.96	0.46
1:A:642:VAL:C	1:A:645:PRO:HD2	2.39	0.46
1:A:1216:ARG:HE	1:B:677:VAL:HG23	1.79	0.46
1:A:1232:LYS:HB3	1:A:1232:LYS:HZ2	1.79	0.46
1:B:373:ALA:O	1:B:376:LYS:HB3	2.15	0.46
1:B:667:LEU:HD12	1:B:667:LEU:N	2.31	0.46
1:B:154:LEU:HD13	1:B:250:VAL:HG22	1.96	0.46
1:A:390:PHE:CE2	1:A:403:LEU:HD22	2.51	0.46
1:A:667:LEU:N	1:A:667:LEU:HD12	2.31	0.46
1:B:694:GLN:O	1:B:698:VAL:HB	2.16	0.46
1:A:373:ALA:O	1:A:376:LYS:HB3	2.15	0.46
1:A:710:LYS:HD2	1:A:734:TYR:CE1	2.51	0.46
1:A:814:GLY:O	1:A:1080:MET:HE3	2.15	0.46
1:B:317:LEU:C	1:B:317:LEU:HD22	2.39	0.46
1:B:390:PHE:CE2	1:B:403:LEU:HD22	2.51	0.46
1:B:693:ASN:HD21	1:B:736:PHE:HZ	1.63	0.46
1:B:1200:THR:HA	1:B:1201:PRO:HD3	1.83	0.46
1:A:184:GLU:CD	1:A:256:ARG:HH12	2.23	0.46
1:A:274:VAL:HG23	1:A:324:ILE:HD12	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:GLN:C	1:A:1048:GLN:NE2	2.73	0.46
1:A:1200:THR:CG2	1:A:1202:MET:H	2.28	0.46
1:A:173:GLY:O	1:A:174:PHE:HB2	2.16	0.46
1:A:684:TRP:HZ2	1:A:689:CYS:SG	2.39	0.46
1:A:917:LYS:NZ	1:A:917:LYS:CB	2.78	0.46
1:A:1007:THR:HB	1:A:1152:VAL:HG22	1.96	0.46
1:A:1040:VAL:HA	1:A:1098:LEU:HD22	1.96	0.46
1:B:93:MET:O	1:B:97:MET:HG3	2.16	0.46
1:B:97:MET:HE1	1:B:133:ALA:HB1	1.98	0.46
1:B:1048:GLN:C	1:B:1048:GLN:NE2	2.73	0.46
1:B:1200:THR:CG2	1:B:1202:MET:H	2.28	0.46
1:A:368:LYS:HZ3	1:B:227:GLN:HE22	1.62	0.46
1:A:820:TYR:HD1	1:A:1049:PHE:CZ	2.34	0.46
1:B:820:TYR:HD1	1:B:1049:PHE:CZ	2.34	0.46
1:A:97:MET:HE1	1:A:133:ALA:HB1	1.98	0.46
1:B:184:GLU:CD	1:B:256:ARG:HH12	2.23	0.46
1:A:694:GLN:O	1:A:698:VAL:HB	2.16	0.46
1:A:1043:GLY:HA2	1:A:1084:GLN:NE2	2.31	0.46
1:A:1219:THR:HB	1:A:1222:GLN:OE1	2.16	0.46
1:B:152:MET:HE3	1:B:303:ARG:HG3	1.98	0.45
1:B:274:VAL:HG23	1:B:324:ILE:HD12	1.98	0.45
1:A:280:CYS:HB3	1:A:301:LYS:HG2	1.99	0.45
1:A:421:GLN:HA	1:A:466:SER:O	2.16	0.45
1:A:644:LYS:N	1:A:645:PRO:CD	2.79	0.45
1:A:1010:VAL:O	1:B:1188:PHE:HB3	2.16	0.45
1:A:1071:CYS:HA	4:A:1235:SF4:S3	2.56	0.45
1:A:1162:GLU:HG3	1:B:1171:ILE:HG21	1.98	0.45
1:B:780:TYR:HA	1:B:783:ARG:HD2	1.99	0.45
1:B:1074:GLN:O	1:B:1133:ARG:HG2	2.16	0.45
1:A:64:GLU:HG3	1:A:89:GLY:CA	2.45	0.45
1:A:198:LYS:O	1:A:202:GLU:HG3	2.17	0.45
1:A:325:THR:HG23	1:A:382:MET:CE	2.47	0.45
1:A:1141:PHE:N	1:A:1142:PRO:HD3	2.31	0.45
1:B:87:SER:HA	1:B:129:ASP:CB	2.46	0.45
1:B:146:VAL:HG21	1:B:179:GLU:O	2.16	0.45
1:B:421:GLN:HA	1:B:466:SER:O	2.16	0.45
1:B:1141:PHE:N	1:B:1142:PRO:HD3	2.31	0.45
1:A:93:MET:O	1:A:97:MET:HG3	2.16	0.45
1:A:208:MET:HE2	1:B:833:PHE:HD2	1.82	0.45
1:A:469:ARG:NH2	1:A:479:TYR:O	2.49	0.45
1:A:1080:MET:H	1:B:1215:ASN:ND2	2.14	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:MET:HG2	1:A:1149:ARG:HE	1.80	0.45
1:B:280:CYS:HB3	1:B:301:LYS:HG2	1.99	0.45
1:B:286:VAL:HG12	1:B:290:LEU:HD22	1.97	0.45
1:B:390:PHE:CG	1:B:403:LEU:HD13	2.51	0.45
1:B:710:LYS:HD2	1:B:734:TYR:CE1	2.51	0.45
1:B:755:CYS:HA	1:B:756:PRO:HD3	1.64	0.45
1:B:1071:CYS:HA	4:B:1242:SF4:S3	2.56	0.45
1:A:617:LYS:HA	1:A:617:LYS:HD3	1.71	0.45
1:A:1074:GLN:O	1:A:1133:ARG:HG2	2.16	0.45
1:B:198:LYS:O	1:B:202:GLU:HG3	2.17	0.45
1:B:469:ARG:NH2	1:B:479:TYR:O	2.49	0.45
1:B:1219:THR:HB	1:B:1222:GLN:OE1	2.16	0.45
1:A:87:SER:HA	1:A:129:ASP:CB	2.47	0.45
1:A:704:ILE:HG12	1:A:740:ILE:CD1	2.47	0.45
1:A:790:VAL:HG13	1:A:791:LEU:N	2.31	0.45
1:B:684:TRP:HZ2	1:B:689:CYS:SG	2.39	0.45
1:B:1059:PHE:HD1	1:B:1104:ARG:CD	2.30	0.45
1:A:87:SER:N	1:A:129:ASP:OD2	2.49	0.45
1:A:124:PHE:CB	1:A:367:SER:HB2	2.26	0.45
1:A:390:PHE:CG	1:A:403:LEU:HD13	2.51	0.45
1:A:467:HIS:C	1:A:468:LEU:HD23	2.42	0.45
1:A:1198:ASP:OD2	1:A:1203:MET:HE3	2.17	0.45
1:B:467:HIS:C	1:B:468:LEU:HD23	2.42	0.45
1:B:704:ILE:HG12	1:B:740:ILE:CD1	2.47	0.45
1:A:210:PRO:CB	1:B:831:ARG:HA	2.47	0.45
1:A:791:LEU:HD23	1:A:791:LEU:HA	1.84	0.45
1:B:14:THR:HG21	1:B:171:PHE:CE1	2.51	0.45
1:B:173:GLY:O	1:B:174:PHE:HB2	2.16	0.45
1:B:512:LEU:HG	1:B:514:SER:HB3	1.98	0.45
1:B:790:VAL:HG13	1:B:791:LEU:N	2.31	0.45
1:A:780:TYR:HA	1:A:783:ARG:HD2	1.99	0.45
1:B:44:ALA:CB	1:B:58:ILE:HD11	2.47	0.45
1:B:87:SER:N	1:B:129:ASP:OD2	2.49	0.45
1:B:887:ARG:NH2	1:B:954:LYS:N	2.65	0.45
1:A:78:GLY:HA2	1:A:207:SER:OG	2.17	0.45
1:A:593:LYS:HD3	1:A:594:LYS:H	1.82	0.45
1:A:755:CYS:SG	1:A:761:ALA:CB	3.02	0.45
1:B:707:VAL:O	1:B:736:PHE:HA	2.17	0.45
1:B:1005:THR:HA	1:B:1006:PRO:HD3	1.71	0.45
1:A:707:VAL:O	1:A:736:PHE:HA	2.17	0.44
1:A:741:ASN:CG	1:A:744:ASP:HB2	2.42	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:GLY:O	1:B:941:LEU:C	2.60	0.44
1:B:1043:GLY:HA2	1:B:1084:GLN:NE2	2.31	0.44
1:A:596:GLU:O	1:A:599:VAL:HB	2.18	0.44
1:A:636:ASN:ND2	1:A:672:PHE:CE2	2.85	0.44
1:A:670:SER:HA	1:A:673:GLU:OE1	2.18	0.44
1:A:940:GLY:O	1:A:941:LEU:C	2.60	0.44
1:A:1108:GLN:H	1:A:1108:GLN:HG2	1.57	0.44
1:B:636:ASN:ND2	1:B:672:PHE:CE2	2.85	0.44
1:A:1059:PHE:HD1	1:A:1104:ARG:CD	2.30	0.44
1:A:44:ALA:CB	1:A:58:ILE:HD11	2.47	0.44
1:A:146:VAL:HG21	1:A:179:GLU:O	2.16	0.44
1:A:152:MET:HE3	1:A:303:ARG:HG3	1.98	0.44
1:A:208:MET:HE1	1:B:879:MET:CE	2.46	0.44
1:A:325:THR:HA	1:A:359:LEU:O	2.18	0.44
1:B:35:THR:O	1:B:36:MET:C	2.61	0.44
1:B:82:THR:HG22	1:B:83:THR:N	2.26	0.44
1:B:644:LYS:N	1:B:645:PRO:CD	2.79	0.44
1:B:741:ASN:CG	1:B:744:ASP:HB2	2.42	0.44
1:A:368:LYS:NZ	1:B:227:GLN:NE2	2.65	0.44
1:A:887:ARG:NH2	1:A:954:LYS:N	2.65	0.44
1:B:124:PHE:HB3	1:B:367:SER:CB	2.28	0.44
1:B:325:THR:HG23	1:B:382:MET:CE	2.47	0.44
1:B:35:THR:O	1:B:38:GLU:N	2.51	0.44
1:B:64:GLU:OE2	5:B:1243:TPP:N1'	2.51	0.44
1:A:263:TYR:OH	1:A:298:GLY:HA3	2.18	0.44
1:A:331:LYS:HE3	1:B:230:GLU:OE2	2.17	0.44
1:A:1219:THR:HG21	1:A:1221:GLU:HG2	2.00	0.44
1:B:140:MET:HE3	1:B:168:MET:SD	2.58	0.44
1:B:523:ASP:HA	1:B:531:LYS:HZ1	1.78	0.44
1:B:593:LYS:HD3	1:B:594:LYS:H	1.82	0.44
1:B:746:MET:HB3	1:B:813:SER:OG	2.18	0.44
1:B:1082:LYS:HD3	1:B:1082:LYS:HA	1.84	0.44
1:B:1219:THR:HG21	1:B:1221:GLU:HG2	2.00	0.44
1:A:512:LEU:HG	1:A:514:SER:HB3	1.98	0.44
1:A:890:LEU:CD1	1:A:945:ILE:HG23	2.45	0.44
1:B:263:TYR:OH	1:B:298:GLY:HA3	2.18	0.44
1:B:698:VAL:HG22	1:B:1084:GLN:CD	2.43	0.44
1:A:805:LEU:HD22	1:A:829:GLY:HA3	2.00	0.44
1:A:843:ILE:HG13	1:A:996:ASN:OD1	2.18	0.44
1:A:1005:THR:HA	1:A:1006:PRO:HD3	1.71	0.44
1:B:596:GLU:O	1:B:599:VAL:HB	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:LEU:HD22	1:B:829:GLY:HA3	2.00	0.44
1:A:140:MET:HE3	1:A:168:MET:SD	2.58	0.43
1:B:803:GLU:O	1:B:805:LEU:HD13	2.18	0.43
1:B:867:SER:HB2	1:B:875:TYR:CD2	2.53	0.43
1:B:843:ILE:HG13	1:B:996:ASN:OD1	2.18	0.43
1:B:1000:GLN:HE21	1:B:1000:GLN:HB2	1.67	0.43
1:B:1198:ASP:OD2	1:B:1203:MET:HE3	2.17	0.43
1:A:746:MET:HB3	1:A:813:SER:OG	2.18	0.43
1:A:754:ILE:O	1:A:755:CYS:C	2.61	0.43
1:B:325:THR:HA	1:B:359:LEU:O	2.18	0.43
1:B:679:ILE:HD13	1:B:679:ILE:HA	1.90	0.43
1:A:64:GLU:OE2	5:A:1236:TPP:N1'	2.51	0.43
1:A:650:GLN:NE2	1:A:653:LYS:NZ	2.66	0.43
1:A:821:VAL:O	1:A:825:THR:HG23	2.18	0.43
1:B:78:GLY:HA2	1:B:207:SER:OG	2.17	0.43
1:B:490:HIS:CD2	1:B:490:HIS:N	2.86	0.43
1:B:650:GLN:NE2	1:B:653:LYS:NZ	2.66	0.43
1:B:670:SER:HA	1:B:673:GLU:OE1	2.18	0.43
1:B:1180:GLY:O	1:B:1181:LYS:HD2	2.19	0.43
1:A:35:THR:O	1:A:38:GLU:N	2.51	0.43
1:A:290:LEU:O	1:A:293:LYS:HB2	2.19	0.43
1:A:593:LYS:CG	1:A:594:LYS:H	2.31	0.43
1:B:290:LEU:O	1:B:293:LYS:HB2	2.19	0.43
1:A:1104:ARG:O	1:A:1107:ALA:HB3	2.18	0.43
1:A:1180:GLY:O	1:A:1181:LYS:HD2	2.19	0.43
1:A:317:LEU:HD21	1:A:321:ALA:CB	2.49	0.43
1:B:591:TYR:HA	1:B:593:LYS:HG2	2.00	0.43
1:B:1104:ARG:O	1:B:1107:ALA:HB3	2.18	0.43
1:A:11:ASN:HD21	1:A:112:THR:HG21	1.84	0.43
1:A:521:ASP:O	1:A:522:MET:C	2.62	0.43
1:A:552:ASP:C	1:A:554:GLY:H	2.27	0.43
1:A:687:GLU:H	1:A:687:GLU:HG3	1.65	0.43
1:A:831:ARG:HA	1:B:210:PRO:HB2	2.01	0.43
1:A:1217:ALA:HB2	1:B:679:ILE:HB	2.01	0.43
1:B:1227:SER:C	1:B:1229:ARG:H	2.27	0.43
1:A:693:ASN:HD21	1:A:736:PHE:HZ	1.63	0.43
1:A:698:VAL:O	1:A:700:PRO:HD3	2.19	0.43
1:A:698:VAL:HG22	1:A:1084:GLN:CD	2.43	0.43
1:A:867:SER:HB2	1:A:875:TYR:CD2	2.53	0.43
1:B:226:PHE:O	1:B:226:PHE:CD1	2.72	0.43
1:B:509:THR:HA	1:B:540:LYS:HB2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:LYS:HD2	1:B:598:ILE:HG13	2.01	0.43
1:B:317:LEU:HD21	1:B:321:ALA:CB	2.49	0.43
1:B:374:MET:O	1:B:377:SER:HB3	2.18	0.43
1:B:698:VAL:O	1:B:700:PRO:HD3	2.19	0.43
1:A:370:PHE:CZ	1:A:375:VAL:HG22	2.54	0.42
1:A:422:PHE:CE1	1:A:468:LEU:HG	2.54	0.42
1:B:212:HIS:O	1:B:212:HIS:CG	2.72	0.42
1:B:346:SER:O	1:B:350:GLU:HB3	2.19	0.42
1:B:370:PHE:CZ	1:B:375:VAL:HG22	2.54	0.42
1:A:19:TYR:CD1	1:A:19:TYR:C	2.97	0.42
1:A:208:MET:HE2	1:B:833:PHE:CD2	2.54	0.42
1:A:630:LYS:H	1:A:630:LYS:HG3	1.57	0.42
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	2.00	0.42
1:A:1227:SER:C	1:A:1229:ARG:H	2.27	0.42
1:B:19:TYR:CD1	1:B:19:TYR:C	2.97	0.42
1:B:154:LEU:HD13	1:B:250:VAL:CG2	2.49	0.42
1:B:266:ALA:HA	1:B:267:PRO:HD3	1.91	0.42
1:B:455:TYR:HB3	1:B:456:ASP:H	1.64	0.42
1:B:511:VAL:CG2	1:B:563:MET:HE1	2.50	0.42
1:B:821:VAL:O	1:B:825:THR:HG23	2.18	0.42
1:A:154:LEU:HD13	1:A:250:VAL:CG2	2.49	0.42
1:A:509:THR:HA	1:A:540:LYS:HB2	2.01	0.42
1:A:511:VAL:HA	1:A:542:TYR:O	2.19	0.42
1:A:792:PRO:O	1:A:793:ARG:C	2.63	0.42
1:A:1205:ARG:HA	1:A:1205:ARG:HD3	1.82	0.42
1:B:390:PHE:HA	1:B:401:THR:O	2.19	0.42
1:B:554:GLY:CA	1:B:601:MET:HE2	2.40	0.42
1:B:593:LYS:CG	1:B:594:LYS:H	2.31	0.42
1:B:897:ALA:HB3	1:B:910:LEU:HD21	2.01	0.42
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.91	0.42
1:A:346:SER:O	1:A:350:GLU:HB3	2.19	0.42
1:A:490:HIS:N	1:A:490:HIS:CD2	2.86	0.42
1:B:64:GLU:CG	1:B:89:GLY:HA2	2.48	0.42
1:B:154:LEU:CD2	1:B:158:LEU:HD11	2.49	0.42
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.82	0.42
1:B:472:GLU:H	1:B:472:GLU:HG2	1.55	0.42
1:B:754:ILE:O	1:B:755:CYS:C	2.61	0.42
1:A:307:PRO:HA	1:B:334:GLY:O	2.19	0.42
1:A:591:TYR:HA	1:A:593:LYS:HG2	2.00	0.42
1:A:897:ALA:HB3	1:A:910:LEU:HD21	2.01	0.42
1:B:536:ASN:ND2	1:B:623:LYS:HG2	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:VAL:O	1:B:602:ASN:HB2	2.20	0.42
1:A:35:THR:O	1:A:36:MET:C	2.61	0.42
1:A:390:PHE:HA	1:A:401:THR:O	2.19	0.42
1:A:803:GLU:O	1:A:805:LEU:HD13	2.18	0.42
1:B:5:MET:HE1	1:B:184:GLU:HB2	2.02	0.42
1:B:736:PHE:CD2	1:B:801:PHE:HZ	2.37	0.42
1:B:792:PRO:O	1:B:793:ARG:C	2.63	0.42
1:B:1094:GLY:HA3	1:B:1120:PRO:HG3	2.00	0.42
1:B:1123:SER:O	1:B:1124:VAL:C	2.63	0.42
1:A:5:MET:HE1	1:A:184:GLU:HB2	2.02	0.42
1:A:374:MET:O	1:A:377:SER:HB3	2.18	0.42
1:A:390:PHE:CD2	1:A:403:LEU:HD22	2.54	0.42
1:A:467:HIS:CE1	1:A:480:LEU:HD22	2.55	0.42
1:A:1082:LYS:HD3	1:A:1082:LYS:HA	1.84	0.42
1:B:11:ASN:HD21	1:B:112:THR:HG21	1.84	0.42
1:B:325:THR:HG22	1:B:382:MET:SD	2.60	0.42
1:B:390:PHE:CD2	1:B:403:LEU:HD22	2.54	0.42
1:B:596:GLU:O	1:B:597:LYS:C	2.62	0.42
1:B:840:CYS:O	1:B:844:TRP:CD1	2.72	0.42
1:B:1108:GLN:H	1:B:1108:GLN:HG2	1.57	0.42
1:A:226:PHE:O	1:A:226:PHE:CD1	2.72	0.42
1:A:511:VAL:CG2	1:A:563:MET:HE1	2.50	0.42
1:A:513:ASN:HA	1:A:544:ILE:O	2.20	0.42
1:A:736:PHE:CD2	1:A:801:PHE:HZ	2.37	0.42
1:A:941:LEU:HA	1:A:941:LEU:HD23	1.86	0.42
1:A:976:HIS:HE1	1:B:60:GLU:O	2.03	0.42
1:B:338:ASP:HB3	1:B:339:PRO:CD	2.50	0.42
1:B:465:ILE:HG13	1:B:467:HIS:HE1	1.84	0.42
1:B:552:ASP:C	1:B:554:GLY:H	2.27	0.42
1:B:687:GLU:H	1:B:687:GLU:HG3	1.65	0.42
1:B:1149:ARG:HG3	1:B:1149:ARG:NH1	2.15	0.42
1:A:64:GLU:CG	1:A:89:GLY:HA2	2.48	0.42
1:A:154:LEU:CD2	1:A:158:LEU:HD11	2.49	0.42
1:A:212:HIS:O	1:A:212:HIS:CG	2.72	0.42
1:A:696:ALA:O	1:A:822:ARG:NH2	2.53	0.42
1:A:840:CYS:O	1:A:844:TRP:CD1	2.72	0.42
1:B:317:LEU:HD21	1:B:321:ALA:HB3	2.02	0.42
1:B:536:ASN:HD22	1:B:623:LYS:HZ3	1.66	0.42
1:B:780:TYR:CE2	1:B:784:ILE:HD11	2.55	0.42
1:B:1132:ASN:ND2	1:B:1139:ARG:HH12	2.11	0.42
1:A:465:ILE:HG13	1:A:467:HIS:HE1	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:LYS:NZ	1:B:1219:THR:HG21	2.34	0.42
1:B:32:PRO:HB3	1:B:174:PHE:CE2	2.55	0.42
1:B:513:ASN:HA	1:B:544:ILE:O	2.20	0.42
1:B:715:VAL:C	1:B:717:ALA:N	2.77	0.42
1:A:32:PRO:HB3	1:A:174:PHE:CE2	2.55	0.41
1:A:227:GLN:HE22	1:B:368:LYS:HZ3	1.68	0.41
1:A:780:TYR:CE2	1:A:784:ILE:HD11	2.55	0.41
1:A:965:TRP:CZ3	1:A:966:ALA:HB2	2.55	0.41
1:B:197:GLN:H	1:B:197:GLN:HG2	1.64	0.41
1:B:467:HIS:CE1	1:B:480:LEU:HD22	2.55	0.41
1:B:630:LYS:H	1:B:630:LYS:HG3	1.57	0.41
1:B:748:CYS:SG	1:B:750:ASN:HB2	2.60	0.41
1:B:837:ALA:HB2	1:B:872:ALA:CB	2.50	0.41
1:A:317:LEU:HD21	1:A:321:ALA:HB3	2.02	0.41
1:A:660:GLU:O	1:A:661:ALA:C	2.63	0.41
1:A:837:ALA:HB2	1:A:872:ALA:CB	2.50	0.41
1:A:1209:GLY:O	1:B:429:GLY:HA2	2.19	0.41
1:B:227:GLN:NE2	1:B:227:GLN:H	2.18	0.41
1:B:1059:PHE:CD1	1:B:1104:ARG:HD3	2.55	0.41
1:A:208:MET:HE1	1:B:879:MET:HE1	2.01	0.41
1:A:748:CYS:SG	1:A:750:ASN:HB2	2.60	0.41
1:A:1132:ASN:ND2	1:A:1139:ARG:HH12	2.11	0.41
1:B:23:GLU:CD	1:B:204:ARG:HH22	2.28	0.41
1:B:371:SER:HB2	1:B:372:PRO:CD	2.51	0.41
1:B:897:ALA:HA	1:B:941:LEU:HD13	2.03	0.41
1:B:965:TRP:CZ3	1:B:966:ALA:HB2	2.55	0.41
1:B:1149:ARG:CG	1:B:1149:ARG:NH1	2.80	0.41
1:A:23:GLU:CD	1:A:204:ARG:HH22	2.28	0.41
1:A:238:LYS:O	1:A:242:ILE:HG13	2.20	0.41
1:A:536:ASN:HA	1:A:623:LYS:HZ3	1.85	0.41
1:A:596:GLU:O	1:A:597:LYS:C	2.62	0.41
1:A:700:PRO:HB3	1:A:819:PRO:HD3	2.02	0.41
1:A:743:LEU:HD23	1:A:743:LEU:HA	1.73	0.41
1:A:1123:SER:O	1:A:1124:VAL:C	2.63	0.41
1:A:1149:ARG:HG3	1:A:1149:ARG:NH1	2.15	0.41
1:B:314:PHE:C	1:B:316:ALA:H	2.27	0.41
1:B:491:ASN:HA	1:B:492:PRO:HD2	1.84	0.41
1:B:644:LYS:HB3	1:B:645:PRO:HD3	2.02	0.41
1:B:1001:SER:HB2	1:B:1011:ALA:HB3	2.01	0.41
1:A:536:ASN:ND2	1:A:623:LYS:HG2	2.34	0.41
1:A:593:LYS:HD2	1:A:598:ILE:HG13	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:THR:HA	1:A:1201:PRO:HD3	1.83	0.41
1:A:371:SER:HB2	1:A:372:PRO:CD	2.50	0.41
1:A:599:VAL:O	1:A:602:ASN:HB2	2.20	0.41
1:A:1215:ASN:HD21	1:B:1080:MET:H	1.68	0.41
1:B:696:ALA:O	1:B:822:ARG:NH2	2.53	0.41
1:B:721:PHE:HD1	1:B:777:ASN:ND2	2.18	0.41
1:A:86:ALA:O	1:A:87:SER:C	2.64	0.41
1:A:210:PRO:O	1:B:860:GLN:HB2	2.19	0.41
1:A:338:ASP:HB3	1:A:339:PRO:CD	2.50	0.41
1:A:349:VAL:HG12	1:B:349:VAL:HG12	2.03	0.41
1:A:715:VAL:C	1:A:717:ALA:N	2.77	0.41
1:A:1001:SER:HB2	1:A:1011:ALA:HB3	2.01	0.41
1:B:700:PRO:HB3	1:B:819:PRO:HD3	2.02	0.41
1:A:477:SER:HB3	1:A:479:TYR:CE1	2.55	0.41
1:A:593:LYS:CD	1:A:594:LYS:H	2.34	0.41
1:A:897:ALA:HA	1:A:941:LEU:HD13	2.03	0.41
1:A:1137:LEU:HD23	1:A:1137:LEU:HA	1.90	0.41
1:B:86:ALA:O	1:B:87:SER:C	2.64	0.41
1:B:477:SER:HB3	1:B:479:TYR:CE1	2.55	0.41
1:B:511:VAL:HA	1:B:542:TYR:O	2.19	0.41
1:B:617:LYS:HA	1:B:617:LYS:HD3	1.71	0.41
1:B:718:PRO:HB2	1:B:777:ASN:HD21	1.86	0.41
5:B:1243:TPP:HN42	5:B:1243:TPP:C2	2.33	0.41
1:A:234:PRO:CA	1:A:237:LEU:HD12	2.44	0.41
1:A:314:PHE:C	1:A:316:ALA:H	2.27	0.41
1:A:325:THR:HG23	1:A:382:MET:HE2	2.03	0.41
1:A:368:LYS:NZ	1:B:223:ASP:O	2.54	0.41
1:A:461:GLY:H	1:B:1214:GLN:CD	2.29	0.41
1:A:644:LYS:HB3	1:A:645:PRO:HD3	2.02	0.41
1:A:804:PRO:HG3	1:A:826:GLN:HE21	1.86	0.41
1:A:879:MET:CE	1:B:208:MET:HE1	2.51	0.41
1:B:226:PHE:CD1	1:B:226:PHE:C	2.99	0.41
1:B:325:THR:HG23	1:B:382:MET:HE2	2.03	0.41
1:B:593:LYS:CD	1:B:594:LYS:H	2.34	0.41
1:B:660:GLU:O	1:B:661:ALA:C	2.63	0.41
5:B:1243:TPP:H2	5:B:1243:TPP:N4'	2.36	0.41
1:A:605:ALA:O	1:A:609:ALA:HB2	2.21	0.41
1:A:821:VAL:HG21	1:A:844:TRP:HH2	1.86	0.41
1:A:875:TYR:CE1	1:B:73:GLY:HA2	2.56	0.41
1:A:1177:PRO:O	1:A:1178:ALA:HB2	2.21	0.41
1:B:346:SER:O	1:B:350:GLU:CB	2.69	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ALA:O	1:B:609:ALA:HB2	2.21	0.41
1:B:619:PRO:HB2	1:B:621:SER:HB3	2.03	0.41
1:B:1177:PRO:O	1:B:1178:ALA:HB2	2.21	0.41
1:A:697:PHE:HD2	1:A:800:GLN:HE21	1.67	0.40
5:A:1236:TPP:H2	5:A:1236:TPP:N4'	2.36	0.40
1:B:853:TYR:CE2	1:B:864:TRP:NE1	2.89	0.40
1:A:24:VAL:CG1	1:B:881:MET:HE2	2.46	0.40
1:A:96:ASN:O	1:A:99:LYS:N	2.55	0.40
1:A:226:PHE:CD1	1:A:226:PHE:C	2.99	0.40
5:A:1236:TPP:HN42	5:A:1236:TPP:C2	2.33	0.40
1:B:96:ASN:O	1:B:99:LYS:N	2.55	0.40
1:B:238:LYS:O	1:B:242:ILE:HG13	2.20	0.40
1:B:273:ILE:HD13	1:B:273:ILE:HG21	1.63	0.40
1:B:755:CYS:HA	4:B:1240:SF4:S1	2.61	0.40
1:B:893:LEU:HD12	1:B:893:LEU:HA	1.88	0.40
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.82	0.40
1:A:619:PRO:HB2	1:A:621:SER:HB3	2.03	0.40
1:A:721:PHE:HD1	1:A:777:ASN:ND2	2.18	0.40
1:A:853:TYR:CE2	1:A:864:TRP:NE1	2.89	0.40
1:A:1146:LYS:HA	1:A:1149:ARG:NH1	2.37	0.40
1:B:755:CYS:SG	1:B:761:ALA:CB	3.02	0.40
1:A:5:MET:CE	1:A:184:GLU:HB2	2.52	0.40
1:A:693:ASN:O	1:A:697:PHE:HB2	2.22	0.40
1:A:755:CYS:HA	4:A:1233:SF4:S1	2.61	0.40
1:B:388:ASN:OD1	1:B:389:HIS:N	2.54	0.40
1:A:718:PRO:HB2	1:A:777:ASN:HD21	1.86	0.40
1:A:856:ASN:HD21	1:A:860:GLN:HG3	1.87	0.40
1:A:1118:LYS:HE3	1:A:1118:LYS:HB2	1.94	0.40
1:B:811:ALA:HB2	1:B:844:TRP:CB	2.52	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:N	1:B:634:MET:CE[3_445]	2.01	0.19
1:A:292:ALA:CA	1:B:634:MET:CE[3_445]	2.05	0.15
1:A:291:ALA:C	1:B:634:MET:CE[3_445]	2.12	0.08
1:A:291:ALA:O	1:B:634:MET:CE[3_445]	2.18	0.02

## 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	1229/1231 (100%)	1101 (90%)	103 (8%)	25 (2%)	6	28
1	B	1229/1231 (100%)	1102 (90%)	102 (8%)	25 (2%)	6	28
All	All	2458/2462 (100%)	2203 (90%)	205 (8%)	50 (2%)	6	28

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	218	THR
1	A	595	GLY
1	A	626	PRO
1	A	627	ALA
1	A	1124	VAL
1	A	1178	ALA
1	A	1231	LYS
1	B	87	SER
1	B	218	THR
1	B	595	GLY
1	B	626	PRO
1	B	627	ALA
1	B	1124	VAL
1	B	1178	ALA
1	B	1231	LYS
1	A	711	GLU
1	A	940	GLY
1	A	941	LEU
1	A	993	VAL
1	A	996	ASN
1	A	1181	LYS
1	B	711	GLU
1	B	940	GLY
1	B	941	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	993	VAL
1	B	996	ASN
1	B	1181	LYS
1	A	356	PRO
1	A	903	SER
1	A	1174	SER
1	B	356	PRO
1	B	903	SER
1	B	1174	SER
1	A	221	ASN
1	A	353	GLU
1	A	364	GLY
1	A	691	GLN
1	A	1182	ALA
1	B	221	ASN
1	B	353	GLU
1	B	364	GLY
1	B	691	GLN
1	B	1182	ALA
1	A	576	PHE
1	A	599	VAL
1	B	576	PHE
1	B	599	VAL
1	A	1179	GLY
1	B	1179	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	978/978 (100%)	818 (84%)	160 (16%)	2	12
1	B	978/978 (100%)	818 (84%)	160 (16%)	2	12
All	All	1956/1956 (100%)	1636 (84%)	320 (16%)	2	12

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	11	ASN
1	A	12	THR
1	A	14	THR
1	A	27	ILE
1	A	58	ILE
1	A	64	GLU
1	A	82	THR
1	A	95	PRO
1	A	111	VAL
1	A	121	LEU
1	A	134	ARG
1	A	141	LEU
1	A	152	MET
1	A	154	LEU
1	A	175	ARG
1	A	180	ILE
1	A	184	GLU
1	A	194	LEU
1	A	198	LYS
1	A	204	ARG
1	A	206	LYS
1	A	211	GLU
1	A	213	PRO
1	A	215	VAL
1	A	218	THR
1	A	227	GLN
1	A	248	GLN
1	A	257	SER
1	A	260	LEU
1	A	273	ILE
1	A	279	SER
1	A	287	ILE
1	A	290	LEU
1	A	302	VAL
1	A	303	ARG
1	A	317	LEU
1	A	324	ILE
1	A	325	THR
1	A	328	ASP
1	A	331	LYS
1	A	342	LEU
1	A	349	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	351	ARG
1	A	357	LYS
1	A	359	LEU
1	A	365	LEU
1	A	367	SER
1	A	392	VAL
1	A	398	VAL
1	A	399	THR
1	A	403	LEU
1	A	415	LYS
1	A	439	LYS
1	A	454	SER
1	A	460	SER
1	A	463	ILE
1	A	465	ILE
1	A	468	LEU
1	A	472	GLU
1	A	482	ASN
1	A	501	LEU
1	A	509	THR
1	A	511	VAL
1	A	512	LEU
1	A	514	SER
1	A	517	SER
1	A	532	ARG
1	A	538	LYS
1	A	570	LEU
1	A	582	LEU
1	A	583	LEU
1	A	593	LYS
1	A	613	LEU
1	A	617	LYS
1	A	621	SER
1	A	628	GLU
1	A	629	THR
1	A	630	LYS
1	A	635	THR
1	A	637	GLU
1	A	643	VAL
1	A	654	LEU
1	A	656	VAL
1	A	673	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	677	VAL
1	A	681	VAL
1	A	683	GLN
1	A	687	GLU
1	A	698	VAL
1	A	702	SER
1	A	710	LYS
1	A	714	LEU
1	A	715	VAL
1	A	718	PRO
1	A	720	ASN
1	A	725	GLU
1	A	730	GLU
1	A	737	ARG
1	A	741	ASN
1	A	771	ARG
1	A	778	LEU
1	A	783	ARG
1	A	800	GLN
1	A	808	PHE
1	A	821	VAL
1	A	823	VAL
1	A	851	MET
1	A	854	LYS
1	A	857	ARG
1	A	858	LEU
1	A	874	GLU
1	A	883	MET
1	A	887	ARG
1	A	910	LEU
1	A	914	LEU
1	A	917	LYS
1	A	921	ILE
1	A	930	LEU
1	A	941	LEU
1	A	942	LEU
1	A	949	SER
1	A	953	THR
1	A	954	LYS
1	A	955	LYS
1	A	986	VAL
1	A	997	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1001	SER
1	A	1002	SER
1	A	1029	VAL
1	A	1048	GLN
1	A	1064	LEU
1	A	1074	GLN
1	A	1104	ARG
1	A	1105	LEU
1	A	1108	GLN
1	A	1110	LYS
1	A	1118	LYS
1	A	1124	VAL
1	A	1126	GLU
1	A	1136	VAL
1	A	1137	LEU
1	A	1146	LYS
1	A	1149	ARG
1	A	1166	MET
1	A	1170	ASN
1	A	1171	ILE
1	A	1173	GLU
1	A	1181	LYS
1	A	1185	SER
1	A	1186	VAL
1	A	1196	THR
1	A	1197	ARG
1	A	1199	ASP
1	A	1200	THR
1	A	1205	ARG
1	A	1219	THR
1	A	1223	GLN
1	A	1225	ASP
1	A	1232	LYS
1	B	7	THR
1	B	11	ASN
1	B	12	THR
1	B	14	THR
1	B	27	ILE
1	B	58	ILE
1	B	64	GLU
1	B	82	THR
1	B	95	PRO

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	111	VAL
1	B	121	LEU
1	B	134	ARG
1	B	141	LEU
1	B	152	MET
1	B	154	LEU
1	B	175	ARG
1	B	180	ILE
1	B	184	GLU
1	B	194	LEU
1	B	198	LYS
1	B	204	ARG
1	B	206	LYS
1	B	211	GLU
1	B	213	PRO
1	B	215	VAL
1	B	218	THR
1	B	227	GLN
1	B	248	GLN
1	B	257	SER
1	B	260	LEU
1	B	273	ILE
1	B	279	SER
1	B	287	ILE
1	B	290	LEU
1	B	302	VAL
1	B	303	ARG
1	B	317	LEU
1	B	324	ILE
1	B	325	THR
1	B	328	ASP
1	B	331	LYS
1	B	342	LEU
1	B	349	VAL
1	B	351	ARG
1	B	357	LYS
1	B	359	LEU
1	B	365	LEU
1	B	367	SER
1	B	392	VAL
1	B	398	VAL
1	B	399	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	403	LEU
1	B	415	LYS
1	B	439	LYS
1	B	454	SER
1	B	460	SER
1	B	463	ILE
1	B	465	ILE
1	B	468	LEU
1	B	472	GLU
1	B	482	ASN
1	B	501	LEU
1	B	509	THR
1	B	511	VAL
1	B	512	LEU
1	B	514	SER
1	B	517	SER
1	B	532	ARG
1	B	538	LYS
1	B	570	LEU
1	B	582	LEU
1	B	583	LEU
1	B	593	LYS
1	B	613	LEU
1	B	617	LYS
1	B	621	SER
1	B	628	GLU
1	B	629	THR
1	B	630	LYS
1	B	635	THR
1	B	637	GLU
1	B	643	VAL
1	B	654	LEU
1	B	656	VAL
1	B	673	GLU
1	B	677	VAL
1	B	681	VAL
1	B	683	GLN
1	B	687	GLU
1	B	698	VAL
1	B	702	SER
1	B	710	LYS
1	B	714	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	715	VAL
1	B	718	PRO
1	B	720	ASN
1	B	725	GLU
1	B	730	GLU
1	B	737	ARG
1	B	741	ASN
1	B	771	ARG
1	B	778	LEU
1	B	783	ARG
1	B	800	GLN
1	B	808	PHE
1	B	821	VAL
1	B	823	VAL
1	B	851	MET
1	B	854	LYS
1	B	857	ARG
1	B	858	LEU
1	B	874	GLU
1	B	883	MET
1	B	887	ARG
1	B	910	LEU
1	B	914	LEU
1	B	917	LYS
1	B	921	ILE
1	B	930	LEU
1	B	941	LEU
1	B	942	LEU
1	B	949	SER
1	B	953	THR
1	B	954	LYS
1	B	955	LYS
1	B	986	VAL
1	B	997	THR
1	B	1001	SER
1	B	1002	SER
1	B	1029	VAL
1	B	1048	GLN
1	B	1064	LEU
1	B	1074	GLN
1	B	1104	ARG
1	B	1105	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1108	GLN
1	B	1110	LYS
1	B	1118	LYS
1	B	1124	VAL
1	B	1126	GLU
1	B	1136	VAL
1	B	1137	LEU
1	B	1146	LYS
1	B	1149	ARG
1	B	1166	MET
1	B	1170	ASN
1	B	1171	ILE
1	B	1173	GLU
1	B	1181	LYS
1	B	1185	SER
1	B	1186	VAL
1	B	1196	THR
1	B	1197	ARG
1	B	1199	ASP
1	B	1200	THR
1	B	1205	ARG
1	B	1219	THR
1	B	1223	GLN
1	B	1225	ASP
1	B	1232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	11	ASN
1	A	16	HIS
1	A	46	GLN
1	A	110	HIS
1	A	147	GLN
1	A	169	HIS
1	A	212	HIS
1	A	220	GLN
1	A	227	GLN
1	A	233	ASN
1	A	288	ASN
1	A	389	HIS
1	A	421	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	434	ASN
1	A	467	HIS
1	A	491	ASN
1	A	536	ASN
1	A	543	ASN
1	A	560	ASN
1	A	636	ASN
1	A	650	GLN
1	A	688	ASN
1	A	693	ASN
1	A	720	ASN
1	A	739	GLN
1	A	741	ASN
1	A	750	ASN
1	A	765	GLN
1	A	777	ASN
1	A	800	GLN
1	A	918	ASN
1	A	976	HIS
1	A	996	ASN
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN
1	A	1088	ASN
1	A	1108	GLN
1	A	1111	ASN
1	A	1132	ASN
1	A	1215	ASN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	110	HIS
1	B	128	GLN
1	B	147	GLN
1	B	169	HIS
1	B	212	HIS
1	B	220	GLN
1	B	227	GLN
1	B	233	ASN
1	B	288	ASN
1	B	389	HIS
1	B	421	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	434	ASN
1	B	467	HIS
1	B	491	ASN
1	B	536	ASN
1	B	543	ASN
1	B	560	ASN
1	B	636	ASN
1	B	650	GLN
1	B	688	ASN
1	B	693	ASN
1	B	720	ASN
1	B	739	GLN
1	B	741	ASN
1	B	750	ASN
1	B	777	ASN
1	B	800	GLN
1	B	918	ASN
1	B	976	HIS
1	B	996	ASN
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1088	ASN
1	B	1108	GLN
1	B	1111	ASN
1	B	1132	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SF4	B	1242	1	0,12,12	-	-	-		
5	TPP	B	1243	2	26,27,27	1.42	5 (19%)	38,40,40	1.89	8 (21%)
4	SF4	A	1235	1	0,12,12	-	-	-		
5	TPP	A	1236	2	26,27,27	1.42	5 (19%)	38,40,40	1.89	8 (21%)
6	PYR	B	1246	-	5,5,5	4.14	3 (60%)	3,6,6	2.84	2 (66%)
4	SF4	B	1240	1	0,12,12	-	-	-		
4	SF4	A	1234	1	0,12,12	-	-	-		
6	PYR	A	1239	-	5,5,5	4.15	3 (60%)	3,6,6	2.83	2 (66%)
4	SF4	B	1241	1	0,12,12	-	-	-		
4	SF4	A	1233	1	0,12,12	-	-	-		

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
4	SF4	B	1242	1	-	-	0/6/5/5
5	TPP	B	1243	2	-	9/17/17/17	0/2/2/2
4	SF4	A	1235	1	-	-	0/6/5/5
6	PYR	B	1246	-	-	0/4/4/4	-
5	TPP	A	1236	2	-	9/17/17/17	0/2/2/2
4	SF4	B	1240	1	-	-	0/6/5/5
4	SF4	A	1234	1	-	-	0/6/5/5
4	SF4	A	1233	1	-	-	0/6/5/5
4	SF4	B	1241	1	-	-	0/6/5/5
6	PYR	A	1239	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1239	PYR	O3-CA	7.81	1.41	1.23
6	B	1246	PYR	O3-CA	7.79	1.40	1.23
6	A	1239	PYR	CA-C	-3.51	1.42	1.54
6	B	1246	PYR	CA-C	-3.49	1.42	1.54
6	B	1246	PYR	O-C	3.38	1.30	1.22
6	A	1239	PYR	O-C	3.38	1.30	1.22
5	B	1243	TPP	C4'-N3'	3.20	1.39	1.35
5	A	1236	TPP	C4'-N3'	3.16	1.39	1.35
5	A	1236	TPP	C2'-N1'	3.00	1.38	1.34
5	B	1243	TPP	C2'-N1'	2.98	1.38	1.34
5	B	1243	TPP	PB-O3B	-2.44	1.45	1.54
5	A	1236	TPP	PB-O3B	-2.44	1.45	1.54
5	A	1236	TPP	C7'-N3	2.38	1.53	1.48
5	B	1243	TPP	C7'-N3	2.38	1.53	1.48
5	B	1243	TPP	PA-O3A	-2.17	1.57	1.59
5	A	1236	TPP	PA-O3A	-2.14	1.57	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1236	TPP	C7'-N3-C2	6.12	136.25	123.48
5	B	1243	TPP	C7'-N3-C2	6.11	136.24	123.48
5	B	1243	TPP	O3B-PB-O2B	3.80	122.06	107.80
5	A	1236	TPP	O3B-PB-O2B	3.80	122.04	107.80
5	B	1243	TPP	C2-N3-C4	-3.72	109.03	114.06
5	A	1236	TPP	C2-N3-C4	-3.72	109.03	114.06
5	A	1236	TPP	CM2-C2'-N1'	3.64	121.08	117.20
5	B	1243	TPP	CM2-C2'-N1'	3.63	121.07	117.20
6	B	1246	PYR	OXT-C-CA	3.46	123.19	113.59
6	A	1239	PYR	OXT-C-CA	3.45	123.16	113.59
6	B	1246	PYR	OXT-C-O	-3.43	115.74	123.90
6	A	1239	PYR	OXT-C-O	-3.42	115.75	123.90
5	A	1236	TPP	C7'-N3-C4	-3.15	114.01	122.36
5	B	1243	TPP	C7'-N3-C4	-3.15	114.02	122.36
5	A	1236	TPP	N1'-C2'-N3'	-2.50	121.37	125.53
5	B	1243	TPP	N1'-C2'-N3'	-2.48	121.40	125.53
5	A	1236	TPP	PA-O7-C7	2.41	132.75	121.26
5	B	1243	TPP	PA-O7-C7	2.41	132.75	121.26
5	A	1236	TPP	C2-S1-C5	-2.21	89.75	91.22
5	B	1243	TPP	C2-S1-C5	-2.21	89.75	91.22

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1236	TPP	C7-O7-PA-O2A
5	A	1236	TPP	C7-O7-PA-O3A
5	A	1236	TPP	PA-O3A-PB-O3B
5	B	1243	TPP	C7-O7-PA-O2A
5	B	1243	TPP	C7-O7-PA-O3A
5	B	1243	TPP	PA-O3A-PB-O3B
5	A	1236	TPP	C5'-C7'-N3-C2
5	B	1243	TPP	C5'-C7'-N3-C2
5	A	1236	TPP	C5-C6-C7-O7
5	B	1243	TPP	C5-C6-C7-O7
5	A	1236	TPP	C7-O7-PA-O1A
5	B	1243	TPP	C7-O7-PA-O1A
5	A	1236	TPP	PB-O3A-PA-O2A
5	B	1243	TPP	PB-O3A-PA-O2A
5	A	1236	TPP	C4'-C5'-C7'-N3
5	B	1243	TPP	C4'-C5'-C7'-N3
5	A	1236	TPP	PB-O3A-PA-O1A
5	B	1243	TPP	PB-O3A-PA-O1A

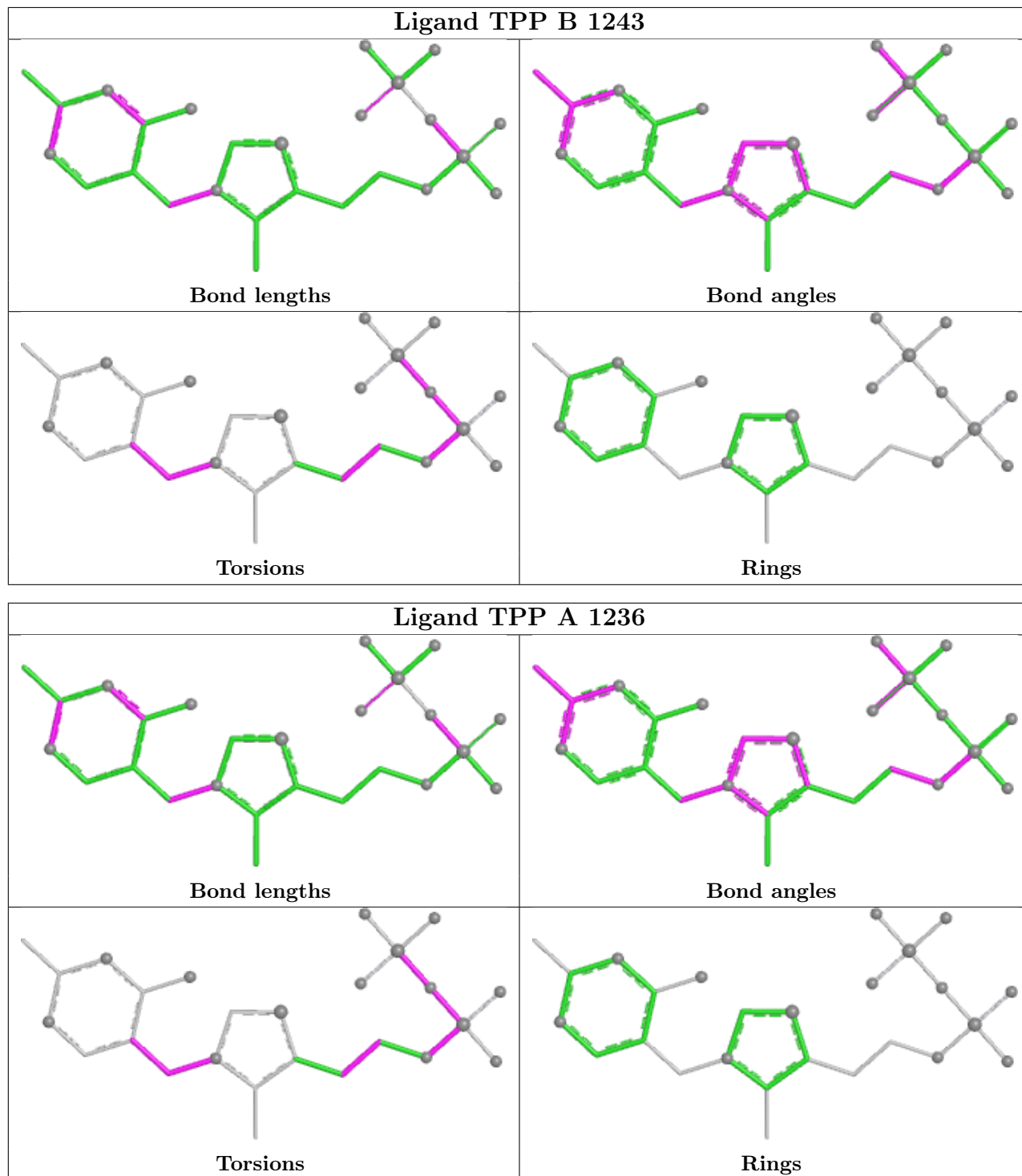
There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1242	SF4	1	0
5	B	1243	TPP	6	0
4	A	1235	SF4	1	0
5	A	1236	TPP	6	0
6	B	1246	PYR	2	0
4	B	1240	SF4	1	0
4	A	1234	SF4	2	0
6	A	1239	PYR	2	0
4	B	1241	SF4	2	0
4	A	1233	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.