



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 1B0P / pdb_00001b0p
Title : CRYSTAL STRUCTURE OF PYRUVATE-FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIBRIO AFRICANUS
Authors : Chabriere, E.; Charon, M.H.; Volbeda, A.
Deposited on : 1998-11-12
Resolution : 2.31 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

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)
Xtriage (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

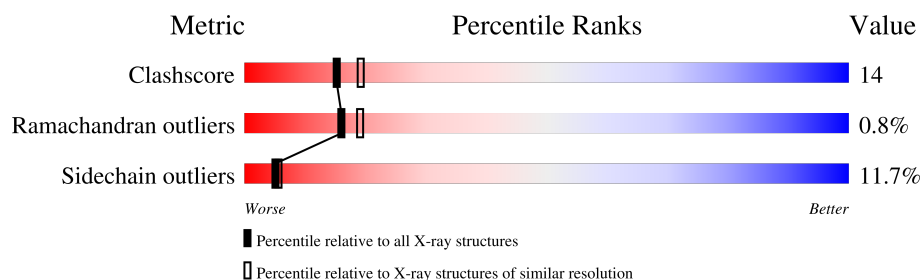
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)

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 ≥ 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	 66% 26% 7%
1	B	1231	 65% 27% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19411 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	0	0	0
			9382	5941	1599	1783	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9382	5941	1599	1783	59			

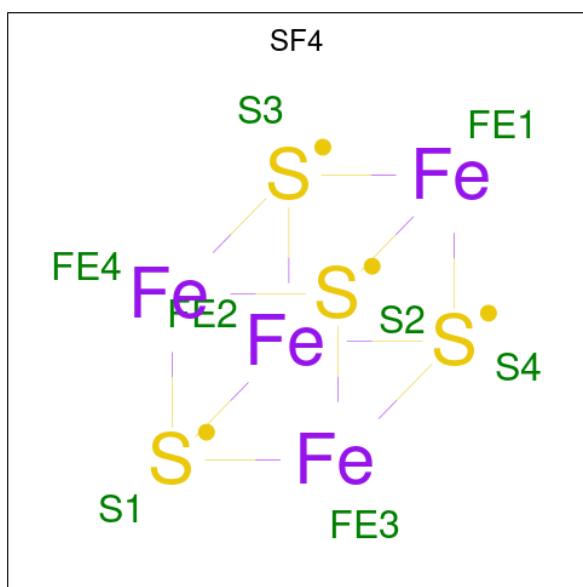
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

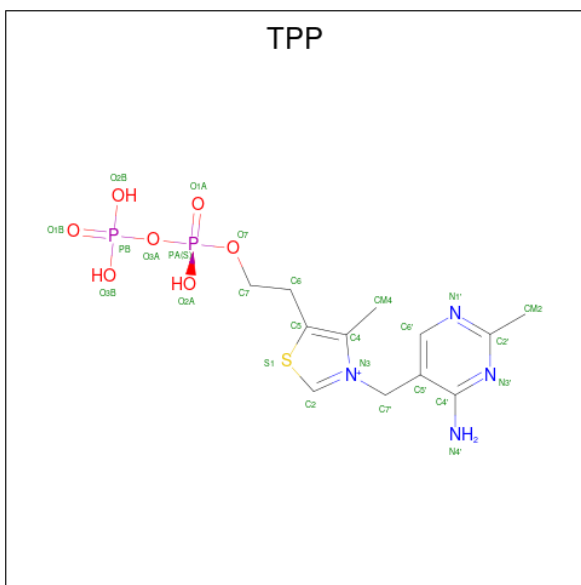
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
5	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 6 is water.

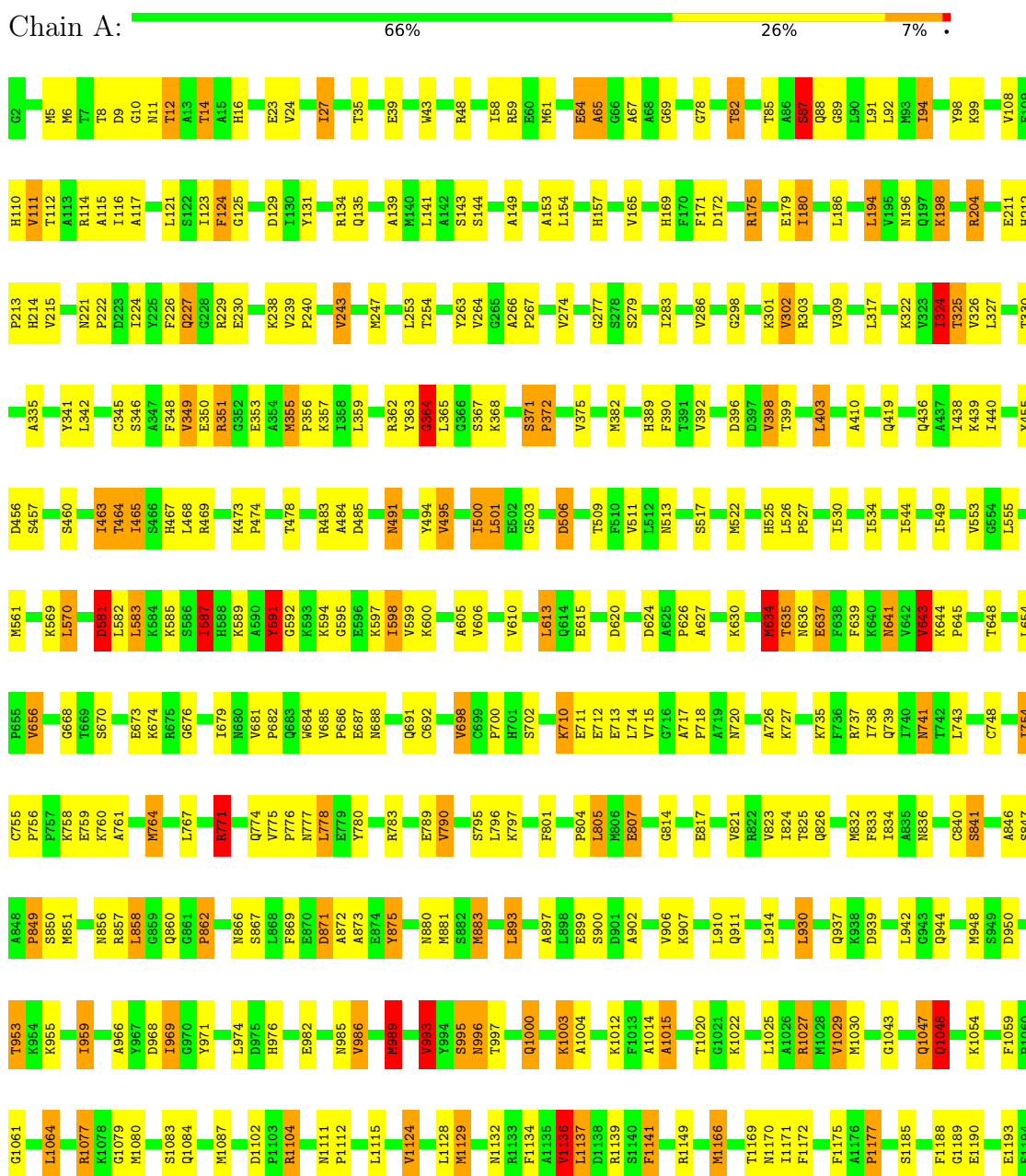
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	273	Total O 273 273	0	0
6	B	270	Total O 270 270	0	0

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.

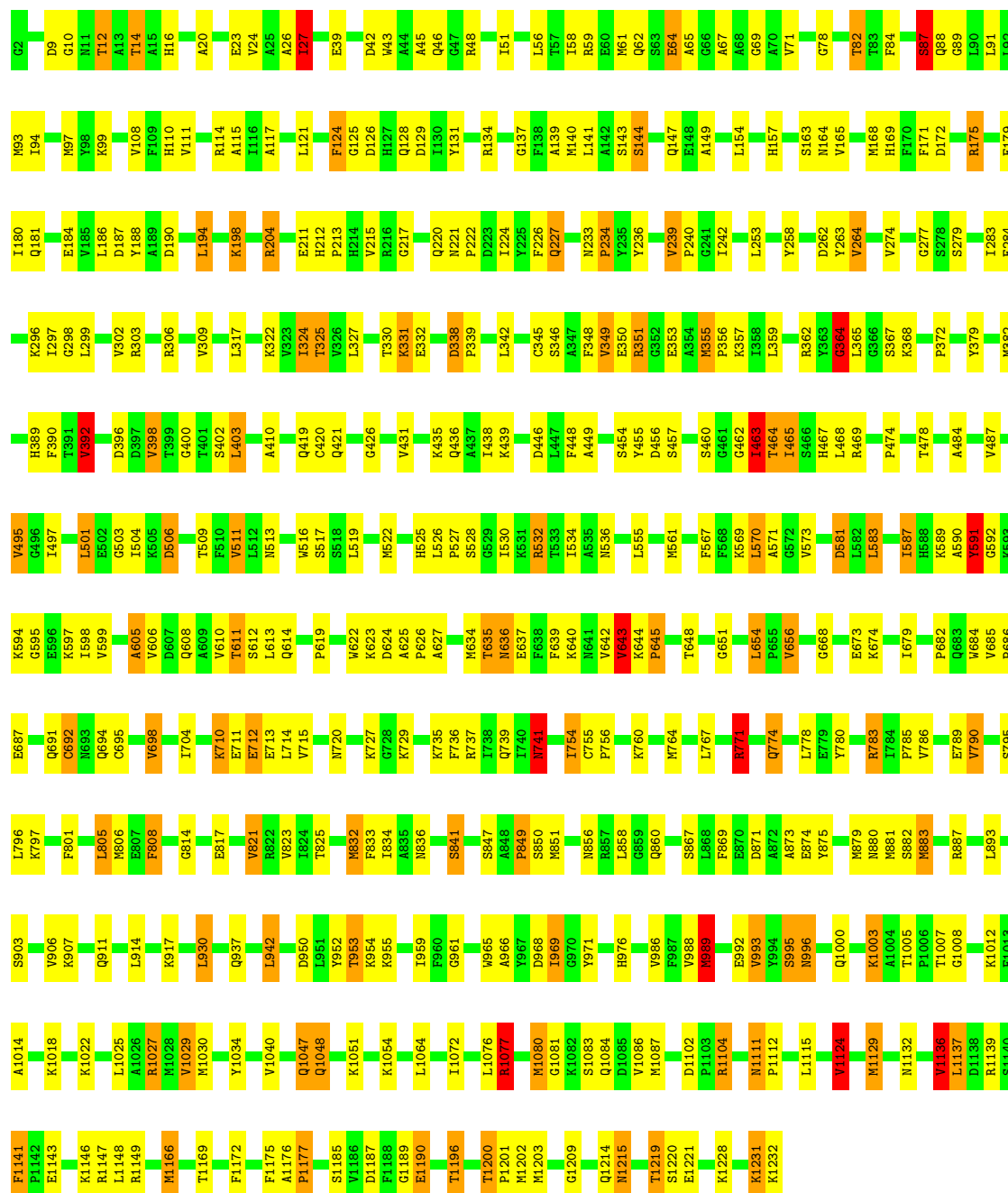
• Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)





● Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)

Chain B: 65% 27% 7%



4 Data and refinement statistics

Xtriage (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, α , β , γ	84.80Å 144.90Å 203.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.31	Depositor
% Data completeness (in resolution range)	68.6 (6.00-2.31)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.854	Depositor
R, R_{free}	0.199 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19411	wwPDB-VP
Average B, all atoms (Å ²)	6.0	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: CA, SF4, TPP, MG

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	0.98	15/9584 (0.2%)	1.30	104/12954 (0.8%)
1	B	0.99	9/9584 (0.1%)	1.29	90/12954 (0.7%)
All	All	0.99	24/19168 (0.1%)	1.30	194/25908 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ILE	CA-CB	9.99	1.59	1.54
1	B	883	MET	SD-CE	-9.43	1.55	1.79
1	A	989	MET	SD-CE	-9.18	1.56	1.79
1	A	948	MET	SD-CE	8.54	2.00	1.79
1	B	165	VAL	CA-C	8.47	1.59	1.53
1	B	1129	MET	SD-CE	-8.20	1.59	1.79
1	A	764	MET	SD-CE	-7.21	1.61	1.79
1	A	883	MET	SD-CE	-7.20	1.61	1.79
1	B	511	VAL	CA-CB	7.18	1.62	1.54
1	B	239	VAL	CA-CB	6.74	1.58	1.53
1	A	165	VAL	CA-CB	6.10	1.61	1.54
1	A	993	VAL	CA-CB	5.83	1.62	1.54
1	A	1129	MET	SD-CE	-5.82	1.65	1.79
1	B	1166	MET	SD-CE	5.67	1.93	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	ILE	CA-CB	5.62	1.62	1.54
1	A	247	MET	SD-CE	-5.55	1.65	1.79
1	A	1166	MET	SD-CE	5.42	1.93	1.79
1	A	309	VAL	CA-CB	5.38	1.60	1.53
1	B	989	MET	SD-CE	-5.26	1.66	1.79
1	B	605	ALA	CA-CB	-5.26	1.45	1.53
1	A	5	MET	SD-CE	5.12	1.92	1.79
1	A	302	VAL	CA-CB	5.12	1.60	1.54
1	B	786	VAL	CA-CB	5.08	1.60	1.54
1	A	180	ILE	CA-CB	5.06	1.60	1.54

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLY	N-CA-C	12.47	128.49	111.03
1	B	756	PRO	N-CA-C	10.80	123.88	110.70
1	B	832	MET	N-CA-C	10.22	126.57	110.32
1	A	756	PRO	N-CA-C	10.17	123.11	110.70
1	A	771	ARG	N-CA-C	9.96	122.13	111.28
1	B	771	ARG	N-CA-C	8.94	121.83	111.11
1	A	27	ILE	N-CA-C	8.91	123.02	109.20
1	A	832	MET	N-CA-C	8.83	124.39	110.17
1	B	969	ILE	N-CA-C	8.71	120.55	110.62
1	A	790	VAL	N-CA-C	8.66	119.45	110.62
1	A	1124	VAL	CB-CA-C	-8.52	101.06	111.97
1	A	1141	PHE	CA-C-N	8.43	128.93	119.32
1	A	1141	PHE	C-N-CA	8.43	128.93	119.32
1	B	1124	VAL	CB-CA-C	-8.34	101.21	111.88
1	B	790	VAL	N-CA-C	8.32	119.11	110.62
1	A	124	PHE	N-CA-C	8.29	121.22	110.53
1	A	627	ALA	N-CA-C	8.25	120.97	110.24
1	B	27	ILE	N-CA-C	8.23	121.96	109.20
1	A	685	VAL	CA-C-N	8.19	128.65	119.32
1	A	685	VAL	C-N-CA	8.19	128.65	119.32
1	B	668	GLY	N-CA-C	8.16	126.64	115.30
1	A	643	VAL	N-CA-C	8.09	118.87	110.62
1	B	402	SER	N-CA-C	8.08	121.89	110.50
1	B	355	MET	CA-C-N	7.94	129.76	119.84
1	B	355	MET	C-N-CA	7.94	129.76	119.84
1	B	643	VAL	N-CA-C	7.92	118.72	110.72
1	A	711	GLU	N-CA-C	7.82	121.76	111.75
1	A	637	GLU	N-CA-C	-7.71	102.81	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	969	ILE	N-CA-C	7.42	119.08	110.62
1	A	995	SER	N-CA-C	7.36	119.20	111.03
1	B	871	ASP	N-CA-C	7.35	122.36	112.88
1	B	65	ALA	N-CA-C	-7.28	103.43	111.36
1	B	591	TYR	N-CA-C	7.25	126.25	110.80
1	B	774	GLN	N-CA-C	7.21	121.83	112.89
1	A	65	ALA	N-CA-C	-7.16	103.52	111.82
1	B	685	VAL	CA-C-N	6.93	128.50	119.84
1	B	685	VAL	C-N-CA	6.93	128.50	119.84
1	A	243	VAL	N-CA-C	-6.87	103.96	110.42
1	A	1015	ALA	N-CA-C	6.87	121.36	113.19
1	A	971	TYR	N-CA-C	6.84	118.74	111.28
1	B	570	LEU	N-CA-C	6.82	122.70	113.97
1	A	774	GLN	N-CA-C	6.81	121.34	112.89
1	B	711	GLU	N-CA-C	6.79	121.16	112.34
1	A	139	ALA	N-CA-C	-6.78	100.45	110.48
1	B	996	ASN	N-CA-C	6.78	118.67	111.28
1	B	172	ASP	N-CA-C	6.77	120.19	110.10
1	B	966	ALA	N-CA-C	6.75	118.64	111.28
1	B	213	PRO	N-CA-C	6.75	121.53	111.41
1	B	801	PHE	N-CA-C	-6.72	105.06	112.72
1	B	1077	ARG	N-CA-C	6.71	120.57	112.38
1	A	570	LEU	N-CA-C	6.68	122.52	113.97
1	B	591	TYR	CA-CB-CG	-6.65	101.93	113.90
1	A	213	PRO	N-CA-C	6.60	121.31	111.41
1	B	1080	MET	N-CA-C	-6.59	105.20	113.18
1	A	668	GLY	N-CA-C	6.59	125.23	115.08
1	A	484	ALA	N-CA-C	6.58	120.59	110.20
1	B	995	SER	N-CA-C	6.55	118.30	111.03
1	A	824	ILE	N-CA-C	-6.55	104.13	110.42
1	A	591	TYR	N-CA-C	6.52	124.69	110.80
1	A	875	TYR	N-CA-C	-6.46	104.32	111.36
1	A	517	SER	N-CA-C	6.44	119.29	111.82
1	A	78	GLY	N-CA-C	6.43	124.98	115.08
1	B	220	GLN	N-CA-C	6.41	119.85	109.40
1	B	525	HIS	N-CA-C	6.40	121.37	113.50
1	A	630	LYS	N-CA-C	6.39	119.62	110.10
1	B	129	ASP	N-CA-C	6.36	118.01	111.14
1	B	679	ILE	N-CA-C	-6.36	104.65	110.82
1	A	679	ILE	N-CA-C	-6.33	104.69	110.82
1	A	125	GLY	N-CA-C	6.31	128.14	113.18
1	A	758	LYS	N-CA-C	-6.31	104.41	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1124	VAL	N-CA-CB	6.25	117.45	110.51
1	B	715	VAL	N-CA-C	6.23	116.90	110.36
1	A	1077	ARG	N-CA-C	6.23	120.14	112.54
1	A	760	LYS	N-CA-C	6.22	119.39	110.24
1	B	612	SER	N-CA-C	6.21	120.99	113.17
1	B	692	CYS	N-CA-C	6.21	120.93	113.23
1	A	1014	ALA	N-CA-C	-6.20	103.10	110.41
1	A	996	ASN	N-CA-C	6.14	118.76	111.33
1	A	748	CYS	N-CA-C	6.12	117.75	111.14
1	B	78	GLY	N-CA-C	6.11	124.50	115.08
1	B	587	ILE	N-CA-C	-6.11	104.79	110.53
1	B	971	TYR	N-CA-C	6.08	117.91	111.28
1	A	756	PRO	CA-C-N	-6.07	113.70	119.90
1	A	756	PRO	C-N-CA	-6.07	113.70	119.90
1	A	87	SER	N-CA-C	6.06	123.71	110.80
1	B	484	ALA	N-CA-C	6.05	119.44	110.48
1	A	410	ALA	N-CA-C	6.02	118.48	110.53
1	B	636	ASN	N-CA-C	-6.00	102.80	110.53
1	B	795	SER	N-CA-C	-5.94	100.61	110.17
1	A	355	MET	CA-C-N	5.93	126.71	120.12
1	A	355	MET	C-N-CA	5.93	126.71	120.12
1	B	875	TYR	N-CA-C	-5.93	104.73	111.07
1	B	262	ASP	N-CA-C	5.91	118.53	108.90
1	B	139	ALA	N-CA-C	-5.90	100.93	110.32
1	A	485	ASP	N-CA-C	-5.88	105.19	112.90
1	A	871	ASP	N-CA-C	5.88	121.23	112.94
1	B	1136	VAL	CB-CA-C	-5.88	104.11	112.22
1	A	1215	ASN	N-CA-C	5.87	119.75	112.24
1	B	519	LEU	N-CA-C	-5.87	105.02	111.82
1	A	69	GLY	N-CA-C	-5.84	105.54	113.37
1	B	847	SER	N-CA-C	-5.82	98.25	108.20
1	B	338	ASP	CA-C-N	5.81	127.10	119.84
1	B	338	ASP	C-N-CA	5.81	127.10	119.84
1	A	224	ILE	N-CA-C	5.80	118.77	113.20
1	A	581	ASP	N-CA-C	-5.79	104.88	111.14
1	A	833	PHE	N-CA-C	-5.79	99.74	109.07
1	B	497	ILE	N-CA-C	5.79	118.75	112.96
1	A	214	HIS	CA-C-N	-5.73	116.08	123.19
1	A	214	HIS	C-N-CA	-5.73	116.08	123.19
1	B	124	PHE	N-CA-C	5.73	118.90	110.59
1	A	525	HIS	N-CA-C	5.72	120.53	113.50
1	A	692	CYS	N-CA-C	5.68	120.49	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ALA	N-CA-C	5.67	118.07	110.35
1	A	715	VAL	N-CA-C	5.67	116.13	110.23
1	A	959	ILE	N-CA-C	-5.66	99.39	107.77
1	B	1014	ALA	N-CA-C	-5.66	101.06	109.83
1	A	1136	VAL	CB-CA-C	-5.65	104.51	112.14
1	B	710	LYS	N-CA-C	-5.64	102.13	110.48
1	B	506	ASP	N-CA-C	-5.64	102.05	110.23
1	A	1171	ILE	CB-CA-C	-5.63	103.27	110.98
1	B	58	ILE	CB-CA-C	-5.58	102.52	110.83
1	A	641	ASN	N-CA-C	5.57	120.19	112.45
1	B	581	ASP	N-CA-C	-5.56	105.12	111.07
1	B	589	LYS	N-CA-C	5.53	116.99	111.07
1	A	500	ILE	CB-CA-C	-5.52	104.81	112.04
1	A	491	ASN	CA-C-N	5.51	125.18	119.56
1	A	491	ASN	C-N-CA	5.51	125.18	119.56
1	A	85	THR	N-CA-C	5.51	115.51	108.24
1	B	69	GLY	N-CA-C	-5.48	106.16	112.73
1	B	637	GLU	N-CA-C	-5.46	105.40	111.36
1	A	862	PRO	N-CA-C	5.46	119.07	110.50
1	A	364	GLY	N-CA-C	5.45	126.09	113.18
1	A	501	LEU	N-CA-C	5.45	119.62	112.92
1	B	87	SER	N-CA-C	5.44	122.38	110.80
1	A	795	SER	N-CA-C	-5.42	101.44	110.17
1	A	944	GLN	N-CA-C	-5.41	105.29	111.14
1	A	966	ALA	N-CA-C	5.41	117.26	111.36
1	A	153	ALA	N-CA-C	-5.41	105.46	111.36
1	B	917	LYS	N-CA-C	5.41	118.68	111.75
1	A	1172	PHE	N-CA-C	5.40	117.46	108.99
1	A	634	MET	N-CA-C	-5.39	103.37	110.43
1	B	501	LEU	N-CA-C	5.37	119.82	113.16
1	A	506	ASP	N-CA-C	-5.36	102.11	110.10
1	B	760	LYS	N-CA-C	5.34	117.83	110.35
1	B	517	SER	N-CA-C	5.34	116.91	111.14
1	B	808	PHE	N-CA-C	5.34	118.75	111.39
1	A	587	ILE	N-CA-C	-5.31	105.67	110.82
1	A	807	GLU	N-CA-C	5.30	117.44	109.23
1	B	642	VAL	N-CA-C	5.30	115.81	111.62
1	A	301	LYS	CA-C-N	-5.30	115.75	122.37
1	A	301	LYS	C-N-CA	-5.30	115.75	122.37
1	B	1215	ASN	N-CA-C	5.28	119.00	112.24
1	A	111	VAL	N-CA-C	5.28	116.08	108.48
1	A	591	TYR	CA-CB-CG	-5.27	104.41	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLU	CA-C-N	5.25	125.55	119.93
1	B	332	GLU	C-N-CA	5.25	125.55	119.93
1	B	679	ILE	CB-CA-C	-5.24	105.17	112.04
1	A	982	GLU	N-CA-C	5.23	118.22	110.48
1	B	1176	ALA	CA-C-N	5.22	126.37	119.84
1	B	1176	ALA	C-N-CA	5.22	126.37	119.84
1	A	801	PHE	N-CA-C	-5.21	106.16	112.88
1	A	129	ASP	N-CA-C	5.21	116.77	111.14
1	A	589	LYS	N-CA-C	5.21	116.95	111.28
1	A	615	GLU	N-CA-C	5.20	117.77	110.23
1	A	172	ASP	N-CA-C	5.20	117.84	110.10
1	A	500	ILE	N-CA-C	5.20	116.54	110.62
1	B	741	ASN	N-CA-C	-5.19	98.84	108.24
1	B	1141	PHE	CA-C-N	5.19	124.63	119.24
1	B	1141	PHE	C-N-CA	5.19	124.63	119.24
1	A	846	ALA	CA-C-N	-5.18	115.31	122.30
1	A	846	ALA	C-N-CA	-5.18	115.31	122.30
1	B	364	GLY	N-CA-C	5.17	125.42	113.18
1	A	974	LEU	N-CA-C	-5.17	105.56	111.14
1	B	1176	ALA	N-CA-C	-5.16	98.48	108.45
1	A	371	SER	N-CA-C	5.16	116.06	110.13
1	B	756	PRO	CA-C-N	-5.16	114.45	119.76
1	B	756	PRO	C-N-CA	-5.16	114.45	119.76
1	B	392	VAL	CB-CA-C	-5.12	102.85	110.33
1	B	224	ILE	N-CA-C	5.11	119.97	109.34
1	A	1020	THR	N-CA-C	-5.10	101.44	109.50
1	B	1209	GLY	N-CA-C	5.10	121.73	114.85
1	A	1198	ASP	N-CA-C	5.09	117.93	109.94
1	A	1207	ASP	N-CA-C	5.08	118.51	112.72
1	B	833	PHE	N-CA-C	-5.08	100.90	109.07
1	A	58	ILE	CB-CA-C	-5.07	103.13	110.63
1	B	463	ILE	N-CA-C	-5.04	104.56	110.05
1	A	1048	GLN	N-CA-C	-5.03	105.99	111.82
1	A	985	ASN	CA-C-N	-5.02	116.96	123.19
1	A	985	ASN	C-N-CA	-5.02	116.96	123.19
1	A	939	ASP	N-CA-C	5.02	117.58	109.40
1	A	598	ILE	N-CA-C	-5.02	105.50	110.62
1	B	1081	GLY	N-CA-C	-5.02	109.15	114.67
1	A	847	SER	N-CA-C	-5.01	100.99	108.96
1	B	735	LYS	N-CA-C	-5.01	101.24	109.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	591	TYR	Sidechain
1	B	1034	TYR	Sidechain
1	B	591	TYR	Sidechain

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	9262	261	0
1	B	9382	0	9262	275	0
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	1	0
4	B	24	0	0	1	0
5	A	26	0	16	1	0
5	B	26	0	16	1	0
6	A	273	0	0	14	0
6	B	270	0	0	20	0
All	All	19411	0	18556	499	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 14.

All (499) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:883:MET:HE2	1:B:955:LYS:HG3	1.41	1.02
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.41	1.00
1:A:64:GLU:HG3	1:A:89:GLY:HA2	1.46	0.95
1:B:635:THR:HG23	1:B:639:PHE:HB3	1.48	0.95
1:B:64:GLU:HG3	1:B:89:GLY:HA2	1.49	0.93
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.55	0.89
6:A:1639:HOH:O	1:B:874:GLU:HB3	1.76	0.85

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:HG3	1.57	0.85
1:B:737:ARG:HH11	1:B:739:GLN:NE2	1.72	0.85
1:B:1132:ASN:O	1:B:1136:VAL:HG22	1.77	0.85
1:B:351:ARG:HD2	1:B:353:GLU:HB2	1.59	0.84
1:B:64:GLU:HG3	1:B:89:GLY:CA	2.09	0.82
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.62	0.82
1:A:398:VAL:HG13	1:A:656:VAL:HG22	1.60	0.82
1:B:396:ASP:HA	1:B:656:VAL:HG13	1.62	0.81
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.61	0.81
1:A:64:GLU:HG3	1:A:89:GLY:CA	2.10	0.81
1:A:1199:ASP:HB3	6:B:1784:HOH:O	1.82	0.80
1:A:841:SER:HB2	6:A:1543:HOH:O	1.82	0.79
1:B:817:GLU:HB3	1:B:989:MET:HE2	1.65	0.78
1:B:841:SER:HB2	6:B:1666:HOH:O	1.81	0.78
1:B:198:LYS:HE2	1:B:198:LYS:H	1.49	0.77
1:A:817:GLU:HB3	1:A:989:MET:HE2	1.64	0.77
1:B:144:SER:HB3	1:B:277:GLY:O	1.85	0.76
1:A:817:GLU:HB3	1:A:989:MET:CE	2.15	0.76
1:A:1102:ASP:OD1	1:A:1104:ARG:HD3	1.86	0.76
1:A:330:THR:O	1:A:362:ARG:HD3	1.86	0.75
1:A:61:MET:HE3	6:A:1639:HOH:O	1.87	0.74
1:A:737:ARG:HH11	1:A:739:GLN:NE2	1.86	0.73
1:A:82:THR:HG22	1:A:108:VAL:O	1.88	0.73
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.34	0.73
1:B:398:VAL:HG13	1:B:656:VAL:HG22	1.70	0.73
1:A:24:VAL:HG13	1:B:881:MET:HE2	1.71	0.73
1:A:856:ASN:HD21	1:A:860:GLN:HE21	1.37	0.71
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.72	0.71
1:B:1166:MET:O	1:B:1169:THR:HG22	1.90	0.71
1:B:1132:ASN:ND2	1:B:1139:ARG:HH22	1.87	0.71
1:B:330:THR:O	1:B:362:ARG:HD3	1.91	0.70
1:A:1132:ASN:ND2	1:A:1139:ARG:HH22	1.89	0.70
1:B:856:ASN:HD21	1:B:860:GLN:HE21	1.39	0.70
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.37	0.70
1:B:850:SER:O	1:B:851:MET:HE2	1.93	0.69
1:A:676:GLY:HA2	6:A:1339:HOH:O	1.92	0.69
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.92	0.69
1:B:10:GLY:O	1:B:14:THR:HG23	1.91	0.69
1:B:43:TRP:HB3	1:B:48:ARG:HD3	1.72	0.69
1:A:635:THR:HG23	1:A:636:ASN:N	2.07	0.69
1:B:227:GLN:H	1:B:227:GLN:HE21	1.39	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:14:THR:HG23	1.93	0.69
1:B:82:THR:HG22	1:B:108:VAL:O	1.91	0.69
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.75	0.69
1:B:737:ARG:NH1	1:B:739:GLN:NE2	2.40	0.69
1:B:1147:ARG:HB3	6:B:1623:HOH:O	1.92	0.68
1:B:817:GLU:HB3	1:B:989:MET:CE	2.23	0.68
1:B:140:MET:HE3	1:B:168:MET:HE3	1.76	0.68
1:A:143:SER:OG	1:A:169:HIS:HE1	1.76	0.68
1:B:737:ARG:NH1	1:B:739:GLN:HE22	1.92	0.68
1:A:274:VAL:HG23	1:A:324:ILE:HD11	1.77	0.66
1:B:561:MET:HE1	1:B:583:LEU:CD2	2.25	0.66
1:B:175:ARG:O	1:B:175:ARG:HD3	1.95	0.66
1:A:227:GLN:H	1:A:227:GLN:HE21	1.44	0.66
1:A:1200:THR:HG23	1:A:1202:MET:H	1.60	0.66
1:A:396:ASP:HA	1:A:656:VAL:HG13	1.78	0.65
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.14	0.65
1:A:325:THR:CG2	1:A:382:MET:SD	2.85	0.65
1:A:643:VAL:HB	1:A:849:PRO:HB2	1.76	0.65
1:A:561:MET:HE1	1:A:583:LEU:HD21	1.77	0.65
1:B:274:VAL:HG23	1:B:324:ILE:HD11	1.78	0.65
1:A:995:SER:O	1:B:1203:MET:HE2	1.96	0.65
1:A:873:ALA:HA	1:A:959:ILE:HD13	1.78	0.64
1:A:907:LYS:O	1:A:911:GLN:HG3	1.97	0.64
1:A:1189:GLY:HA3	1:A:1196:THR:HG21	1.79	0.64
1:B:274:VAL:HG23	1:B:324:ILE:CD1	2.26	0.64
1:A:398:VAL:HG13	1:A:656:VAL:CG2	2.27	0.64
1:B:1102:ASP:OD1	1:B:1104:ARG:HD3	1.97	0.64
1:A:131:TYR:O	1:A:134:ARG:HB2	1.97	0.64
1:B:233:ASN:HB2	1:B:234:PRO:HD3	1.78	0.64
1:B:264:VAL:HG11	1:B:284:GLU:HG3	1.80	0.64
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.79	0.63
1:B:279:SER:O	1:B:283:ILE:HG13	1.98	0.63
1:B:635:THR:HG22	1:B:636:ASN:O	1.97	0.63
1:A:196:ASN:OD1	1:A:198:LYS:HE2	1.98	0.63
1:A:263:TYR:OH	1:A:298:GLY:HA3	1.99	0.63
1:B:635:THR:CG2	1:B:639:PHE:HB3	2.26	0.63
1:A:867:SER:O	1:B:99:LYS:HE3	1.99	0.63
1:B:364:GLY:HA2	1:B:368:LYS:HB3	1.81	0.62
1:B:1005:THR:HB	1:B:1018:LYS:HD3	1.81	0.62
1:B:131:TYR:O	1:B:134:ARG:HB2	2.00	0.62
1:A:698:VAL:HG22	1:A:1084:GLN:CD	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:THR:HG22	1:B:149:ALA:HB1	1.82	0.62
1:B:606:VAL:O	1:B:610:VAL:HG23	1.99	0.62
1:B:530:ILE:O	1:B:534:ILE:HG13	1.99	0.61
1:A:390:PHE:HB2	1:A:403:LEU:HD13	1.81	0.61
1:A:682:PRO:HB3	1:A:764:MET:HE1	1.82	0.61
1:A:1189:GLY:CA	1:A:1196:THR:HG21	2.30	0.61
1:A:986:VAL:HG22	1:A:1064:LEU:HD23	1.81	0.61
1:B:907:LYS:O	1:B:911:GLN:HG3	2.00	0.61
1:B:1189:GLY:HA3	1:B:1196:THR:HG21	1.81	0.61
1:A:463:ILE:HG12	1:A:464:THR:N	2.16	0.61
1:A:1129:MET:HE3	1:A:1149:ARG:CZ	2.30	0.61
1:B:1083:SER:O	1:B:1087:MET:HG3	2.01	0.60
1:A:325:THR:HG23	1:A:382:MET:SD	2.41	0.60
1:A:836:ASN:OD1	1:A:841:SER:HB3	2.01	0.60
1:A:227:GLN:H	1:A:227:GLN:NE2	2.00	0.60
1:A:64:GLU:CG	1:A:89:GLY:HA2	2.26	0.60
1:B:698:VAL:HG22	1:B:1084:GLN:CD	2.27	0.60
1:A:1080:MET:H	1:B:1215:ASN:ND2	1.98	0.60
1:A:883:MET:HE2	1:A:955:LYS:CG	2.31	0.60
1:A:274:VAL:HG23	1:A:324:ILE:CD1	2.32	0.60
1:A:356:PRO:O	1:A:357:LYS:HB3	2.02	0.60
1:A:1215:ASN:ND2	1:B:1080:MET:H	2.00	0.60
1:B:163:SER:O	1:B:164:ASN:HB2	2.01	0.60
1:A:279:SER:O	1:A:283:ILE:HG13	2.02	0.59
1:A:636:ASN:HB3	1:A:639:PHE:H	1.67	0.59
1:B:465:ILE:HG13	1:B:467:HIS:CE1	2.37	0.59
1:A:634:MET:SD	1:A:635:THR:N	2.75	0.59
1:B:463:ILE:HG12	1:B:464:THR:N	2.16	0.59
1:B:1025:LEU:O	1:B:1029:VAL:HG13	2.03	0.59
1:A:61:MET:HG3	1:A:67:ALA:HA	1.83	0.59
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.01	0.59
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.84	0.59
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.33	0.59
1:B:396:ASP:HA	1:B:656:VAL:CG1	2.32	0.59
1:B:968:ASP:OD1	1:B:1003:LYS:HB2	2.02	0.59
1:A:881:MET:HE3	1:B:59:ARG:HG2	1.85	0.58
1:A:881:MET:HE2	1:B:24:VAL:HG13	1.85	0.58
1:A:99:LYS:HE3	1:B:867:SER:O	2.03	0.58
1:A:221:ASN:HB3	1:A:222:PRO:HD2	1.85	0.58
1:A:710:LYS:HG2	1:A:713:GLU:OE1	2.04	0.57
1:B:456:ASP:OD2	1:B:463:ILE:HG22	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:HG11	1:A:341:TYR:HA	1.84	0.57
1:B:9:ASP:OD1	1:B:12:THR:HG23	2.04	0.57
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.86	0.57
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.19	0.57
1:A:322:LYS:O	1:A:356:PRO:O	2.22	0.57
1:A:635:THR:HG23	1:A:636:ASN:H	1.68	0.57
1:B:419:GLN:OE1	1:B:469:ARG:NH1	2.37	0.57
1:B:64:GLU:CG	1:B:89:GLY:HA2	2.31	0.57
1:A:117:ALA:HB1	1:B:99:LYS:HE2	1.86	0.57
1:A:438:ILE:HD11	1:A:468:LEU:HD22	1.87	0.57
1:A:239:VAL:CG1	1:A:240:PRO:HD3	2.35	0.56
1:A:691:GLN:HE22	1:A:727:LYS:H	1.53	0.56
1:A:968:ASP:OD1	1:A:1003:LYS:HB2	2.05	0.56
1:A:1004:ALA:O	1:A:1022:LYS:HG3	2.05	0.56
1:A:1083:SER:O	1:A:1087:MET:HG3	2.05	0.56
1:B:9:ASP:HA	1:B:179:GLU:O	2.05	0.56
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.87	0.56
1:A:544:ILE:HD12	1:A:613:LEU:HD13	1.87	0.56
1:B:1137:LEU:HD22	1:B:1141:PHE:HD2	1.71	0.56
1:A:12:THR:HB	1:A:39:GLU:OE2	2.04	0.56
1:A:238:LYS:NZ	6:A:1773:HOH:O	2.39	0.56
1:A:9:ASP:HA	1:A:179:GLU:O	2.06	0.56
1:A:906:VAL:O	1:A:910:LEU:HB2	2.06	0.56
1:B:396:ASP:O	1:B:400:GLY:HA2	2.05	0.55
1:B:61:MET:HG3	1:B:67:ALA:HA	1.88	0.55
1:B:1029:VAL:HG12	6:B:1629:HOH:O	2.06	0.55
1:A:348:PHE:O	1:A:355:MET:HE1	2.06	0.55
1:B:91:LEU:HA	1:B:94:ILE:HD12	1.88	0.55
1:B:1132:ASN:HD22	1:B:1139:ARG:HH22	1.55	0.55
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.89	0.54
1:B:227:GLN:H	1:B:227:GLN:NE2	2.05	0.54
1:B:1000:GLN:HA	1:B:1012:LYS:HB2	1.88	0.54
1:B:1189:GLY:CA	1:B:1196:THR:HG21	2.38	0.54
1:A:1027:ARG:HA	1:A:1030:MET:HE3	1.88	0.54
1:B:619:PRO:HG2	1:B:622:TRP:CD1	2.42	0.54
1:A:436:GLN:O	1:A:440:ILE:HG13	2.07	0.54
1:B:1200:THR:CG2	1:B:1202:MET:HE3	2.38	0.54
1:A:691:GLN:NE2	1:A:727:LYS:H	2.06	0.54
1:A:561:MET:HE2	1:A:606:VAL:HG22	1.89	0.53
1:A:1132:ASN:HD22	1:A:1139:ARG:HH22	1.55	0.53
1:B:595:GLY:C	1:B:597:LYS:H	2.16	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1137:LEU:CD2	1:B:1141:PHE:HD2	2.20	0.53
1:A:364:GLY:HA2	1:A:368:LYS:HB3	1.89	0.53
1:A:456:ASP:OD2	1:A:463:ILE:HG22	2.09	0.53
1:B:12:THR:HB	1:B:39:GLU:OE2	2.08	0.53
1:B:1027:ARG:HA	1:B:1030:MET:HE3	1.90	0.53
1:B:1047:GLN:NE2	6:B:1590:HOH:O	2.42	0.53
1:A:561:MET:HE1	1:A:583:LEU:CD2	2.39	0.53
1:A:737:ARG:HH11	1:A:739:GLN:HE22	1.55	0.53
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.91	0.53
1:A:755:CYS:SG	1:A:761:ALA:HB3	2.48	0.53
1:B:639:PHE:CD1	1:B:643:VAL:HG22	2.44	0.53
1:B:390:PHE:HB2	1:B:403:LEU:HD13	1.91	0.53
1:B:691:GLN:O	1:B:797:LYS:HE3	2.09	0.53
1:B:767:LEU:O	1:B:771:ARG:HG2	2.09	0.53
1:B:814:GLY:O	1:B:1080:MET:HE3	2.08	0.53
1:A:350:GLU:OE1	1:B:389:HIS:HE1	1.92	0.52
1:A:1137:LEU:CD2	1:A:1141:PHE:HD2	2.22	0.52
1:A:175:ARG:HD2	1:A:478:THR:HB	1.91	0.52
1:B:644:LYS:HB3	1:B:645:PRO:HD3	1.90	0.52
1:B:438:ILE:HD11	1:B:468:LEU:HD22	1.91	0.52
1:A:389:HIS:HE1	1:B:350:GLU:OE1	1.92	0.52
1:A:780:TYR:HA	1:A:783:ARG:HH11	1.75	0.52
1:A:1132:ASN:HD21	1:A:1139:ARG:HH12	1.58	0.52
1:A:1175:PHE:CZ	1:A:1177:PRO:HA	2.45	0.52
1:B:1129:MET:HE3	1:B:1149:ARG:CZ	2.40	0.52
1:A:325:THR:HG21	6:A:1560:HOH:O	2.08	0.52
1:A:1202:MET:O	1:A:1205:ARG:NH2	2.42	0.52
1:B:639:PHE:CE1	1:B:643:VAL:HG22	2.45	0.52
1:B:780:TYR:O	1:B:783:ARG:HG3	2.10	0.52
1:B:1219:THR:HG22	1:B:1221:GLU:H	1.75	0.51
1:A:850:SER:O	1:A:851:MET:HE2	2.11	0.51
1:B:495:VAL:HG13	1:B:527:PRO:HD3	1.92	0.51
1:B:691:GLN:HE22	1:B:727:LYS:H	1.58	0.51
1:B:1147:ARG:CB	6:B:1623:HOH:O	2.52	0.51
1:A:419:GLN:OE1	1:A:469:ARG:NH1	2.43	0.51
1:A:682:PRO:HB3	1:A:764:MET:CE	2.41	0.51
1:A:817:GLU:HB3	1:A:989:MET:HE3	1.92	0.51
1:B:16:HIS:HE1	1:B:186:LEU:O	1.94	0.51
1:B:953:THR:HG22	6:B:1425:HOH:O	2.10	0.51
1:B:390:PHE:CD1	1:B:403:LEU:HD22	2.46	0.51
1:B:115:ALA:HB2	1:B:126:ASP:OD2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:CD	1:B:353:GLU:HB2	2.36	0.51
1:B:555:LEU:HD12	1:B:605:ALA:HB2	1.93	0.51
1:B:684:TRP:CE3	1:B:686:PRO:HG3	2.45	0.51
1:B:869:PHE:CD2	1:B:969:ILE:HG21	2.46	0.51
1:A:227:GLN:HE21	1:A:227:GLN:N	2.07	0.51
1:A:1166:MET:O	1:A:1169:THR:HG22	2.11	0.51
1:B:1219:THR:HG22	1:B:1221:GLU:N	2.26	0.51
1:A:1025:LEU:O	1:A:1029:VAL:HG13	2.11	0.50
1:A:1111:ASN:HD22	1:A:1112:PRO:HD2	1.75	0.50
1:B:14:THR:HG21	1:B:171:PHE:CE1	2.46	0.50
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.77	0.50
1:B:573:VAL:HG22	6:B:1532:HOH:O	2.11	0.50
1:B:1146:LYS:HD3	6:B:1649:HOH:O	2.10	0.50
1:A:6:MET:HE3	1:A:8:THR:HG21	1.94	0.50
1:A:702:SER:CB	1:A:807:GLU:HG2	2.42	0.50
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	2.10	0.50
1:B:421:GLN:HE21	1:B:487:VAL:HG22	1.77	0.50
1:B:1008:GLY:HA2	1:B:1148:LEU:HD13	1.92	0.50
1:B:1200:THR:HG23	1:B:1202:MET:H	1.76	0.50
1:B:239:VAL:CG1	1:B:240:PRO:HD3	2.40	0.50
1:B:258:TYR:HD2	6:B:1635:HOH:O	1.94	0.50
1:B:1129:MET:HE3	1:B:1149:ARG:HD3	1.93	0.50
1:B:23:GLU:OE1	1:B:204:ARG:NH2	2.45	0.50
1:B:348:PHE:O	1:B:355:MET:HE1	2.11	0.50
1:B:754:ILE:HG12	6:B:1410:HOH:O	2.12	0.50
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.60	0.50
1:A:1129:MET:HE3	1:A:1149:ARG:NE	2.27	0.50
1:B:110:HIS:CD2	1:B:169:HIS:HD2	2.22	0.50
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.47	0.50
1:B:1175:PHE:CZ	1:B:1177:PRO:HA	2.47	0.49
1:A:254:THR:HG22	6:A:1738:HOH:O	2.12	0.49
1:B:712:GLU:CD	1:B:712:GLU:H	2.20	0.49
1:B:992:GLU:O	1:B:993:VAL:HB	2.12	0.49
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.92	0.49
1:B:522:MET:O	1:B:526:LEU:HB2	2.11	0.49
1:A:345:CYS:O	1:A:349:VAL:HG13	2.13	0.49
1:A:522:MET:O	1:A:526:LEU:HB2	2.13	0.49
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.94	0.49
1:B:1040:VAL:HG12	1:B:1048:GLN:HE22	1.78	0.49
1:A:950:ASP:OD2	1:B:212:HIS:HE1	1.95	0.49
1:A:1215:ASN:HA	6:A:1641:HOH:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.47	0.49
1:A:230:GLU:OE2	1:B:331:LYS:HE3	2.12	0.49
1:A:1203:MET:HE2	1:B:995:SER:O	2.12	0.49
1:B:448:PHE:CZ	1:B:474:PRO:HG3	2.47	0.49
1:B:571:ALA:HB3	6:B:1532:HOH:O	2.12	0.49
1:A:144:SER:HB3	1:A:277:GLY:O	2.12	0.49
1:A:194:LEU:HD21	1:A:253:LEU:HD12	1.94	0.48
1:A:239:VAL:HG13	1:A:240:PRO:HD3	1.94	0.48
1:A:867:SER:HB2	1:A:875:TYR:CD2	2.47	0.48
1:A:530:ILE:O	1:A:534:ILE:HG13	2.14	0.48
1:B:93:MET:O	1:B:97:MET:HG3	2.12	0.48
1:B:883:MET:HE2	1:B:955:LYS:CG	2.28	0.48
1:B:691:GLN:HG2	1:B:736:PHE:CD1	2.48	0.48
1:B:1147:ARG:CG	6:B:1623:HOH:O	2.61	0.48
1:A:390:PHE:CB	1:A:403:LEU:HD13	2.44	0.48
1:A:702:SER:OG	1:A:807:GLU:HG2	2.14	0.48
1:B:23:GLU:CD	1:B:204:ARG:HH22	2.21	0.48
1:A:494:TYR:HB3	1:A:500:ILE:HD11	1.96	0.48
1:B:345:CYS:O	1:B:349:VAL:HG13	2.14	0.48
1:B:1129:MET:HE3	1:B:1149:ARG:NE	2.28	0.48
1:A:1048:GLN:NE2	6:A:1370:HOH:O	2.47	0.48
1:A:691:GLN:O	1:A:797:LYS:HE3	2.13	0.47
1:A:121:LEU:HD23	1:A:121:LEU:C	2.39	0.47
1:A:561:MET:CE	1:A:587:ILE:HD11	2.45	0.47
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.95	0.47
1:A:99:LYS:HE2	1:B:117:ALA:HB1	1.95	0.47
1:B:147:GLN:HE22	1:B:184:GLU:H	1.62	0.47
1:A:1137:LEU:HD22	1:A:1141:PHE:HD2	1.79	0.47
1:B:961:GLY:HA3	1:B:965:TRP:CE3	2.49	0.47
1:A:16:HIS:HE1	1:A:186:LEU:O	1.97	0.47
1:B:741:ASN:C	1:B:741:ASN:HD22	2.23	0.47
1:B:755:CYS:HA	4:B:1233:SF4:S1	2.54	0.47
1:A:737:ARG:NH1	1:A:739:GLN:HE22	2.12	0.47
1:B:239:VAL:HG13	1:B:240:PRO:HD3	1.95	0.47
1:B:263:TYR:OH	1:B:298:GLY:HA3	2.15	0.47
1:B:754:ILE:O	1:B:755:CYS:C	2.58	0.47
1:B:836:ASN:OD1	1:B:841:SER:HB3	2.15	0.47
1:A:365:LEU:HD22	1:B:226:PHE:CD1	2.50	0.47
1:A:569:LYS:HD2	1:A:610:VAL:HG13	1.95	0.47
1:B:20:ALA:HB2	1:B:188:TYR:CE1	2.50	0.47
1:B:463:ILE:HG12	1:B:464:THR:H	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:TRP:O	1:B:522:MET:HE2	2.14	0.47
1:B:1147:ARG:HD2	6:B:1689:HOH:O	2.14	0.47
5:B:1236:TPP:H2	5:B:1236:TPP:HN42	1.78	0.47
1:A:644:LYS:O	1:A:648:THR:HG23	2.15	0.47
1:A:1185:SER:HB3	1:B:45:ALA:HB1	1.96	0.47
1:B:561:MET:HE2	1:B:587:ILE:HD11	1.97	0.47
1:B:695:CYS:HB2	1:B:704:ILE:HD13	1.97	0.47
1:A:483:ARG:HA	1:A:503:GLY:O	2.15	0.46
1:A:1185:SER:HB3	1:B:45:ALA:CB	2.44	0.46
1:B:426:GLY:N	1:B:462:GLY:O	2.49	0.46
1:B:713:GLU:OE1	1:B:785:PRO:HD2	2.16	0.46
1:A:620:ASP:HB3	6:A:1653:HOH:O	2.15	0.46
1:B:635:THR:HG21	1:B:639:PHE:HD2	1.81	0.46
1:B:1196:THR:HB	6:B:1583:HOH:O	2.14	0.46
1:A:143:SER:HB2	1:A:171:PHE:HB3	1.96	0.46
1:A:495:VAL:HG13	1:A:527:PRO:HD3	1.97	0.46
1:A:637:GLU:HG2	1:A:641:ASN:ND2	2.31	0.46
1:A:419:GLN:HG2	1:A:469:ARG:HG2	1.97	0.46
1:A:87:SER:HB2	1:A:116:ILE:HD13	1.96	0.46
1:A:114:ARG:HG2	1:A:115:ALA:N	2.31	0.46
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.13	0.46
1:A:491:ASN:C	1:A:491:ASN:HD22	2.24	0.46
1:B:1048:GLN:NE2	6:B:1507:HOH:O	2.48	0.46
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.83	0.46
1:B:325:THR:CG2	1:B:382:MET:SD	3.04	0.46
1:B:673:GLU:O	1:B:674:LYS:C	2.59	0.46
1:B:163:SER:HB3	1:B:242:ILE:HD12	1.98	0.46
1:B:832:MET:HE2	1:B:834:ILE:HD11	1.97	0.46
1:A:635:THR:CG2	1:A:636:ASN:N	2.74	0.45
1:A:1043:GLY:HA3	1:A:1084:GLN:O	2.15	0.45
1:A:857:ARG:HG3	1:A:858:LEU:HD13	1.98	0.45
1:B:42:ASP:O	1:B:46:GLN:HG3	2.15	0.45
1:A:286:VAL:HG21	1:A:372:PRO:HA	1.97	0.45
1:B:635:THR:CG2	1:B:636:ASN:N	2.79	0.45
1:A:739:GLN:NE2	1:A:777:ASN:HB3	2.32	0.45
1:A:636:ASN:HB2	1:A:639:PHE:HB2	1.99	0.45
1:A:805:LEU:HB2	1:A:825:THR:HB	1.98	0.45
1:B:431:VAL:CG1	1:B:435:LYS:HE3	2.46	0.45
1:B:598:ILE:O	1:B:599:VAL:C	2.60	0.45
1:A:365:LEU:HD22	1:B:226:PHE:CE1	2.52	0.45
1:B:26:ALA:HB3	1:B:71:VAL:HG23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:GLY:O	1:B:654:LEU:HB2	2.17	0.45
1:A:367:SER:HB2	1:B:222:PRO:HG3	1.97	0.45
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.81	0.45
1:B:1077:ARG:HH22	1:B:1139:ARG:HH21	1.65	0.45
1:A:869:PHE:CD2	1:A:969:ILE:HG21	2.52	0.44
1:B:20:ALA:O	1:B:51:ILE:HG12	2.16	0.44
1:B:325:THR:HG21	6:B:1645:HOH:O	2.17	0.44
1:B:692:CYS:SG	1:B:694:GLN:HG3	2.57	0.44
1:B:887:ARG:NH2	1:B:952:TYR:O	2.48	0.44
1:A:555:LEU:HD12	1:A:605:ALA:HB2	1.98	0.44
1:B:1111:ASN:HD22	1:B:1112:PRO:HD2	1.83	0.44
1:B:879:MET:O	1:B:882:SER:HB3	2.18	0.44
1:B:1214:GLN:HG2	1:B:1214:GLN:O	2.18	0.44
1:A:229:ARG:HE	1:B:128:GLN:HE22	1.64	0.44
1:A:595:GLY:C	1:A:597:LYS:H	2.26	0.44
1:A:871:ASP:O	1:A:872:ALA:C	2.61	0.44
1:A:1027:ARG:HG3	1:A:1030:MET:HE3	2.00	0.44
1:A:1200:THR:HG21	6:B:1702:HOH:O	2.17	0.44
1:A:134:ARG:HD2	6:A:1659:HOH:O	2.18	0.44
1:A:1200:THR:HG21	1:A:1202:MET:HE3	2.00	0.44
1:A:1200:THR:CG2	1:A:1202:MET:HE3	2.47	0.44
1:B:236:TYR:O	1:B:239:VAL:HG12	2.18	0.44
1:A:11:ASN:HD21	1:A:112:THR:HG21	1.83	0.44
1:B:10:GLY:O	1:B:14:THR:CG2	2.63	0.44
1:A:10:GLY:O	1:A:14:THR:CG2	2.64	0.44
1:A:897:ALA:C	1:A:899:GLU:H	2.25	0.44
1:B:137:GLY:O	1:B:236:TYR:OH	2.29	0.44
1:B:390:PHE:CE1	1:B:403:LEU:HD22	2.52	0.44
1:B:1072:ILE:HA	6:B:1662:HOH:O	2.17	0.44
1:A:9:ASP:OD1	1:A:12:THR:CG2	2.66	0.44
1:A:738:ILE:HD13	1:A:738:ILE:HA	1.93	0.44
1:A:741:ASN:HA	1:A:778:LEU:HG	1.99	0.44
1:A:1047:GLN:H	1:A:1047:GLN:NE2	2.15	0.44
1:A:1198:ASP:OD1	1:A:1200:THR:HG22	2.16	0.44
1:B:1129:MET:HE3	1:B:1149:ARG:CD	2.48	0.44
1:A:670:SER:HA	1:A:673:GLU:HG3	1.99	0.43
1:A:717:ALA:HA	1:A:718:PRO:HD3	1.91	0.43
1:A:866:ASN:HB3	1:B:217:GLY:O	2.18	0.43
1:A:900:SER:C	1:A:902:ALA:H	2.26	0.43
1:B:1076:LEU:HD13	1:B:1086:VAL:HG21	1.99	0.43
1:A:390:PHE:CD1	1:A:403:LEU:HD22	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:HA	1:A:656:VAL:CG1	2.48	0.43
1:B:322:LYS:O	1:B:356:PRO:O	2.35	0.43
1:B:1027:ARG:HG3	1:B:1030:MET:HE3	1.98	0.43
1:B:1187:ASP:O	1:B:1190:GLU:HB2	2.18	0.43
1:A:997:THR:OG1	1:A:1000:GLN:NE2	2.49	0.43
1:B:640:LYS:HE2	1:B:640:LYS:HB2	1.79	0.43
1:A:356:PRO:O	1:A:357:LYS:CB	2.65	0.43
1:B:87:SER:OG	1:B:88:GLN:N	2.52	0.43
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.48	0.43
1:B:1124:VAL:HG22	6:B:1263:HOH:O	2.18	0.43
1:B:937:GLN:HG2	1:B:942:LEU:HB3	2.00	0.43
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.84	0.43
1:B:806:MET:HE2	1:B:821:VAL:HG22	1.99	0.43
1:B:930:LEU:HD12	1:B:930:LEU:HA	1.85	0.43
1:A:87:SER:OG	1:A:88:GLN:N	2.51	0.43
1:A:549:ILE:O	1:A:553:VAL:HG22	2.19	0.43
1:A:684:TRP:CE3	1:A:686:PRO:HG3	2.54	0.43
1:A:755:CYS:HA	4:A:1233:SF4:S1	2.59	0.43
1:B:569:LYS:HD2	1:B:610:VAL:HG13	2.00	0.43
1:B:808:PHE:CD1	1:B:808:PHE:N	2.86	0.43
1:A:325:THR:HG22	1:A:382:MET:SD	2.57	0.43
1:A:398:VAL:HG23	1:A:399:THR:HG23	2.01	0.43
1:A:1219:THR:HG22	1:A:1221:GLU:N	2.33	0.43
5:A:1236:TPP:H2	5:A:1236:TPP:N4'	2.34	0.43
1:B:390:PHE:CE1	1:B:392:VAL:HG22	2.54	0.43
1:A:953:THR:HG22	6:A:1288:HOH:O	2.18	0.43
1:A:1193:GLU:OE1	1:B:1077:ARG:HB2	2.18	0.43
1:B:14:THR:CG2	1:B:149:ALA:HB1	2.46	0.43
1:B:263:TYR:HA	1:B:299:LEU:O	2.19	0.43
1:A:513:ASN:HA	1:A:544:ILE:O	2.19	0.42
1:A:581:ASP:O	1:A:585:LYS:HG3	2.20	0.42
1:A:771:ARG:O	1:A:775:VAL:HG23	2.19	0.42
1:B:187:ASP:HB2	1:B:190:ASP:OD1	2.19	0.42
1:A:351:ARG:HD2	1:A:353:GLU:HB2	2.01	0.42
1:A:673:GLU:O	1:A:674:LYS:C	2.62	0.42
1:B:532:ARG:HD2	1:B:625:ALA:H	1.83	0.42
1:A:23:GLU:CD	1:A:204:ARG:HH22	2.27	0.42
1:A:467:HIS:HE1	6:A:1671:HOH:O	2.02	0.42
1:A:598:ILE:O	1:A:599:VAL:C	2.62	0.42
1:B:194:LEU:HD21	1:B:253:LEU:HD12	2.01	0.42
1:A:9:ASP:OD1	1:A:12:THR:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:TYR:HA	1:A:783:ARG:HD2	2.01	0.42
1:A:930:LEU:HD12	1:A:930:LEU:HA	1.74	0.42
1:B:240:PRO:HB3	1:B:309:VAL:HG21	2.01	0.42
1:B:438:ILE:HG23	1:B:449:ALA:HB1	2.01	0.42
1:B:805:LEU:HB2	1:B:825:THR:HB	2.02	0.42
1:B:528:SER:HB3	1:B:626:PRO:O	2.20	0.42
1:A:35:THR:O	1:A:39:GLU:HG3	2.20	0.42
1:A:65:ALA:HB2	1:A:92:LEU:HB3	2.02	0.42
1:A:700:PRO:HG2	1:A:814:GLY:HA2	2.02	0.42
1:A:754:ILE:O	1:A:755:CYS:C	2.62	0.42
1:A:754:ILE:HD12	1:A:754:ILE:HA	1.76	0.42
1:B:454:SER:HB2	1:B:465:ILE:HG23	2.01	0.42
1:A:239:VAL:O	1:A:243:VAL:HG23	2.19	0.42
1:B:264:VAL:CG1	1:B:284:GLU:HG3	2.46	0.42
1:B:297:ILE:HB	1:B:379:TYR:CE1	2.55	0.42
1:A:684:TRP:CH2	1:A:737:ARG:HA	2.54	0.42
1:B:108:VAL:HG21	1:B:157:HIS:HA	2.02	0.42
1:B:739:GLN:OE1	1:B:774:GLN:NE2	2.53	0.42
1:A:473:LYS:O	1:A:474:PRO:C	2.63	0.42
1:A:1188:PHE:CE1	1:A:1196:THR:HG23	2.54	0.42
1:B:682:PRO:HB3	1:B:764:MET:CE	2.50	0.42
1:A:365:LEU:HB2	1:B:226:PHE:CG	2.55	0.41
1:A:555:LEU:CD1	1:A:605:ALA:HB2	2.50	0.41
1:A:775:VAL:N	1:A:776:PRO:HD2	2.35	0.41
1:B:536:ASN:ND2	1:B:623:LYS:HG2	2.35	0.41
1:A:226:PHE:CD1	1:B:365:LEU:HD22	2.55	0.41
1:B:296:LYS:HD3	1:B:296:LYS:HA	1.80	0.41
1:B:503:GLY:O	1:B:504:ILE:C	2.62	0.41
1:B:567:PHE:CD1	1:B:571:ALA:HB2	2.56	0.41
1:B:1219:THR:CG2	1:B:1220:SER:N	2.83	0.41
1:A:123:ILE:HD11	1:B:1201:PRO:HB2	2.03	0.41
1:A:229:ARG:HE	1:B:128:GLN:NE2	2.18	0.41
1:A:279:SER:HB3	1:A:363:TYR:HE2	1.85	0.41
1:A:910:LEU:HD12	1:A:930:LEU:HD21	2.01	0.41
1:A:1195:CYS:HB2	6:A:1541:HOH:O	2.19	0.41
1:B:9:ASP:OD1	1:B:12:THR:CG2	2.67	0.41
1:A:688:ASN:HB3	1:A:759:GLU:O	2.20	0.41
1:B:532:ARG:HG3	1:B:623:LYS:O	2.19	0.41
1:A:465:ILE:HG13	1:A:467:HIS:CE1	2.56	0.41
1:A:681:VAL:HG11	1:A:767:LEU:HD13	2.03	0.41
1:A:976:HIS:CG	1:B:62:GLN:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ALA:HB2	1:B:188:TYR:CE2	2.55	0.41
1:B:274:VAL:CG2	1:B:324:ILE:HD11	2.49	0.41
1:A:91:LEU:HA	1:A:94:ILE:HD12	2.02	0.41
1:A:335:ALA:HA	1:B:306:ARG:NE	2.35	0.41
1:A:1003:LYS:HZ2	1:B:976:HIS:HD2	1.68	0.41
1:B:338:ASP:HB3	1:B:339:PRO:CD	2.50	0.41
1:A:858:LEU:HD12	1:A:858:LEU:HA	1.86	0.41
1:B:27:ILE:HD11	1:B:84:PHE:CD2	2.56	0.41
1:B:356:PRO:O	1:B:357:LYS:HB3	2.21	0.41
1:B:644:LYS:O	1:B:648:THR:HG23	2.20	0.41
1:B:992:GLU:HG2	1:B:1022:LYS:NZ	2.35	0.41
1:A:834:ILE:HD12	1:A:862:PRO:HB3	2.02	0.41
1:A:881:MET:HE3	1:B:59:ARG:CG	2.51	0.41
1:A:1199:ASP:O	1:B:455:TYR:HB3	2.20	0.41
1:B:561:MET:CE	1:B:587:ILE:HD11	2.50	0.41
1:A:741:ASN:HD22	1:A:741:ASN:C	2.29	0.41
1:A:743:LEU:HA	1:A:743:LEU:HD23	1.75	0.41
1:A:1059:PHE:CE2	1:A:1061:GLY:HA3	2.55	0.41
1:A:1079:GLY:HA2	1:B:1215:ASN:HD21	1.85	0.41
1:B:131:TYR:CE1	1:B:339:PRO:HB2	2.56	0.41
1:B:227:GLN:HE21	1:B:227:GLN:N	2.11	0.41
1:B:338:ASP:HB3	1:B:339:PRO:HD2	2.03	0.41
1:B:695:CYS:HB2	1:B:704:ILE:CD1	2.51	0.41
1:A:804:PRO:HA	1:A:826:GLN:HG3	2.03	0.41
1:A:1128:LEU:O	1:A:1134:PHE:HB2	2.21	0.41
1:B:608:GLN:HA	1:B:611:THR:OG1	2.20	0.41
1:B:1143:GLU:HB2	1:B:1147:ARG:NH2	2.36	0.41
1:A:1129:MET:HE3	1:A:1149:ARG:HD3	2.03	0.40
1:B:114:ARG:HG2	1:B:115:ALA:N	2.35	0.40
1:B:961:GLY:O	1:B:988:VAL:HA	2.21	0.40
1:A:59:ARG:HG2	1:B:881:MET:HE3	2.04	0.40
1:A:893:LEU:HA	1:A:893:LEU:HD12	1.84	0.40
1:B:121:LEU:C	1:B:121:LEU:HD23	2.47	0.40
1:B:175:ARG:HD2	1:B:478:THR:HB	2.03	0.40
1:B:639:PHE:CE1	1:B:643:VAL:CG2	3.05	0.40
1:A:98:TYR:OH	1:A:135:GLN:HG2	2.21	0.40
1:B:1012:LYS:HA	1:B:1012:LYS:HD2	1.76	0.40
1:A:14:THR:CG2	1:A:149:ALA:HB1	2.52	0.40
1:B:1111:ASN:HA	1:B:1172:PHE:CE1	2.56	0.40
1:A:371:SER:O	1:A:375:VAL:HG23	2.21	0.40
1:B:903:SER:OG	1:B:906:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1229/1231 (100%)	1177 (96%)	43 (4%)	9 (1%)	18	22
1	B	1229/1231 (100%)	1184 (96%)	35 (3%)	10 (1%)	16	19
All	All	2458/2462 (100%)	2361 (96%)	78 (3%)	19 (1%)	16	19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	1231	LYS
1	B	87	SER
1	B	594	LYS
1	B	1231	LYS
1	A	594	LYS
1	A	1177	PRO
1	B	590	ALA
1	B	592	GLY
1	B	627	ALA
1	B	993	VAL
1	A	591	TYR
1	A	592	GLY
1	A	626	PRO
1	B	591	TYR
1	B	1177	PRO
1	B	364	GLY
1	A	364	GLY
1	A	993	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	978/978 (100%)	871 (89%)	107 (11%)	6	7
1	B	978/978 (100%)	857 (88%)	121 (12%)	4	5
All	All	1956/1956 (100%)	1728 (88%)	228 (12%)	5	5

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	14	THR
1	A	27	ILE
1	A	64	GLU
1	A	82	THR
1	A	111	VAL
1	A	141	LEU
1	A	154	LEU
1	A	175	ARG
1	A	180	ILE
1	A	194	LEU
1	A	198	LYS
1	A	204	ARG
1	A	211	GLU
1	A	215	VAL
1	A	227	GLN
1	A	264	VAL
1	A	302	VAL
1	A	303	ARG
1	A	317	LEU
1	A	324	ILE
1	A	325	THR
1	A	327	LEU
1	A	342	LEU
1	A	346	SER
1	A	349	VAL
1	A	351	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	359	LEU
1	A	372	PRO
1	A	392	VAL
1	A	398	VAL
1	A	403	LEU
1	A	439	LYS
1	A	457	SER
1	A	460	SER
1	A	463	ILE
1	A	464	THR
1	A	465	ILE
1	A	495	VAL
1	A	501	LEU
1	A	506	ASP
1	A	509	THR
1	A	511	VAL
1	A	570	LEU
1	A	581	ASP
1	A	582	LEU
1	A	583	LEU
1	A	587	ILE
1	A	600	LYS
1	A	613	LEU
1	A	624	ASP
1	A	634	MET
1	A	635	THR
1	A	643	VAL
1	A	654	LEU
1	A	656	VAL
1	A	687	GLU
1	A	698	VAL
1	A	710	LYS
1	A	712	GLU
1	A	714	LEU
1	A	720	ASN
1	A	735	LYS
1	A	741	ASN
1	A	754	ILE
1	A	771	ARG
1	A	778	LEU
1	A	789	GLU
1	A	790	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	796	LEU
1	A	805	LEU
1	A	821	VAL
1	A	823	VAL
1	A	840	CYS
1	A	841	SER
1	A	849	PRO
1	A	858	LEU
1	A	880	ASN
1	A	893	LEU
1	A	914	LEU
1	A	930	LEU
1	A	953	THR
1	A	986	VAL
1	A	989	MET
1	A	993	VAL
1	A	996	ASN
1	A	1000	GLN
1	A	1003	LYS
1	A	1027	ARG
1	A	1029	VAL
1	A	1047	GLN
1	A	1048	GLN
1	A	1054	LYS
1	A	1064	LEU
1	A	1077	ARG
1	A	1104	ARG
1	A	1115	LEU
1	A	1124	VAL
1	A	1136	VAL
1	A	1137	LEU
1	A	1170	ASN
1	A	1190	GLU
1	A	1196	THR
1	A	1200	THR
1	A	1219	THR
1	A	1231	LYS
1	A	1232	LYS
1	B	12	THR
1	B	14	THR
1	B	27	ILE
1	B	56	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	64	GLU
1	B	82	THR
1	B	111	VAL
1	B	141	LEU
1	B	143	SER
1	B	144	SER
1	B	154	LEU
1	B	175	ARG
1	B	180	ILE
1	B	181	GLN
1	B	194	LEU
1	B	198	LYS
1	B	204	ARG
1	B	211	GLU
1	B	215	VAL
1	B	227	GLN
1	B	234	PRO
1	B	264	VAL
1	B	302	VAL
1	B	303	ARG
1	B	317	LEU
1	B	324	ILE
1	B	325	THR
1	B	327	LEU
1	B	331	LYS
1	B	342	LEU
1	B	346	SER
1	B	349	VAL
1	B	351	ARG
1	B	359	LEU
1	B	372	PRO
1	B	392	VAL
1	B	398	VAL
1	B	403	LEU
1	B	420	CYS
1	B	436	GLN
1	B	439	LYS
1	B	446	ASP
1	B	457	SER
1	B	460	SER
1	B	463	ILE
1	B	464	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	465	ILE
1	B	495	VAL
1	B	501	LEU
1	B	506	ASP
1	B	509	THR
1	B	511	VAL
1	B	513	ASN
1	B	532	ARG
1	B	570	LEU
1	B	581	ASP
1	B	583	LEU
1	B	611	THR
1	B	613	LEU
1	B	614	GLN
1	B	624	ASP
1	B	634	MET
1	B	635	THR
1	B	643	VAL
1	B	645	PRO
1	B	654	LEU
1	B	656	VAL
1	B	687	GLU
1	B	698	VAL
1	B	710	LYS
1	B	712	GLU
1	B	714	LEU
1	B	720	ASN
1	B	729	LYS
1	B	741	ASN
1	B	754	ILE
1	B	771	ARG
1	B	778	LEU
1	B	783	ARG
1	B	789	GLU
1	B	790	VAL
1	B	796	LEU
1	B	805	LEU
1	B	821	VAL
1	B	823	VAL
1	B	841	SER
1	B	849	PRO
1	B	858	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	880	ASN
1	B	893	LEU
1	B	914	LEU
1	B	930	LEU
1	B	942	LEU
1	B	953	THR
1	B	954	LYS
1	B	986	VAL
1	B	989	MET
1	B	996	ASN
1	B	1003	LYS
1	B	1007	THR
1	B	1027	ARG
1	B	1029	VAL
1	B	1047	GLN
1	B	1048	GLN
1	B	1051	LYS
1	B	1054	LYS
1	B	1064	LEU
1	B	1077	ARG
1	B	1104	ARG
1	B	1111	ASN
1	B	1115	LEU
1	B	1124	VAL
1	B	1136	VAL
1	B	1137	LEU
1	B	1190	GLU
1	B	1196	THR
1	B	1200	THR
1	B	1219	THR
1	B	1228	LYS
1	B	1231	LYS
1	B	1232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	110	HIS
1	A	128	GLN
1	A	147	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	ASN
1	A	169	HIS
1	A	212	HIS
1	A	227	GLN
1	A	288	ASN
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	482	ASN
1	A	491	ASN
1	A	513	ASN
1	A	536	ASN
1	A	588	HIS
1	A	602	ASN
1	A	650	GLN
1	A	691	GLN
1	A	693	ASN
1	A	720	ASN
1	A	739	GLN
1	A	741	ASN
1	A	765	GLN
1	A	774	GLN
1	A	777	ASN
1	A	860	GLN
1	A	866	ASN
1	A	880	ASN
1	A	918	ASN
1	A	976	HIS
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN
1	A	1073	ASN
1	A	1088	ASN
1	A	1108	GLN
1	A	1111	ASN
1	A	1132	ASN
1	A	1151	GLN
1	A	1154	HIS
1	A	1215	ASN
1	B	11	ASN
1	B	16	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	46	GLN
1	B	96	ASN
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	288	ASN
1	B	389	HIS
1	B	407	ASN
1	B	421	GLN
1	B	434	ASN
1	B	467	HIS
1	B	482	ASN
1	B	491	ASN
1	B	513	ASN
1	B	536	ASN
1	B	543	ASN
1	B	588	HIS
1	B	602	ASN
1	B	636	ASN
1	B	688	ASN
1	B	691	GLN
1	B	693	ASN
1	B	720	ASN
1	B	739	GLN
1	B	741	ASN
1	B	750	ASN
1	B	770	GLN
1	B	774	GLN
1	B	777	ASN
1	B	860	GLN
1	B	866	ASN
1	B	880	ASN
1	B	976	HIS
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1073	ASN
1	B	1084	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1088	ASN
1	B	1111	ASN
1	B	1132	ASN
1	B	1215	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 [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	1233	1	0,12,12	-	-	-		
4	SF4	B	1234	1	0,12,12	-	-	-		
5	TPP	A	1236	2	26,27,27	1.44	4 (15%)	38,40,40	1.84	10 (26%)
5	TPP	B	1236	2	26,27,27	1.61	5 (19%)	38,40,40	1.53	8 (21%)
4	SF4	B	1235	1	0,12,12	-	-	-		
4	SF4	A	1235	1	0,12,12	-	-	-		
4	SF4	A	1234	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	1233	1	-	-	0/6/5/5
4	SF4	A	1234	1	-	-	0/6/5/5
4	SF4	B	1234	1	-	-	0/6/5/5
5	TPP	A	1236	2	-	7/17/17/17	0/2/2/2
5	TPP	B	1236	2	-	8/17/17/17	0/2/2/2
4	SF4	B	1235	1	-	-	0/6/5/5
4	SF4	A	1235	1	-	-	0/6/5/5
4	SF4	A	1233	1	-	-	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1236	TPP	PA-O3A	-4.25	1.54	1.59
5	B	1236	TPP	PB-O3B	-3.82	1.40	1.54
5	B	1236	TPP	C4'-N3'	3.62	1.39	1.35
5	B	1236	TPP	C2'-N1'	2.53	1.38	1.34
5	A	1236	TPP	PA-O2A	-2.43	1.44	1.55
5	B	1236	TPP	C7'-N3	2.40	1.53	1.48
5	A	1236	TPP	PB-O3B	-2.30	1.46	1.54
5	A	1236	TPP	C7'-N3	2.09	1.53	1.48
5	B	1236	TPP	C2-S1	-2.02	1.62	1.69

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1236	TPP	C2-S1-C5	-5.44	87.61	91.22
5	A	1236	TPP	O3B-PB-O2B	3.57	121.19	107.80
5	B	1236	TPP	O3B-PB-O2B	3.51	120.96	107.80
5	A	1236	TPP	C7'-N3-C4	3.13	130.66	122.36
5	B	1236	TPP	S1-C2-N3	2.97	116.06	112.30
5	B	1236	TPP	CM2-C2'-N1'	2.95	120.34	117.20
5	A	1236	TPP	CM2-C2'-N1'	2.91	120.30	117.20
5	B	1236	TPP	PA-O7-C7	2.79	134.54	121.26
5	A	1236	TPP	N1'-C2'-N3'	-2.73	120.98	125.53
5	B	1236	TPP	C7'-N3-C4	2.65	129.38	122.36
5	A	1236	TPP	C2-N3-C4	-2.61	110.54	114.06
5	A	1236	TPP	PA-O7-C7	2.60	133.62	121.26
5	A	1236	TPP	C5'-C7'-N3	-2.59	107.40	112.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1236	TPP	N1'-C2'-N3'	-2.40	121.54	125.53
5	B	1236	TPP	C7'-N3-C2	-2.31	118.67	123.48
5	A	1236	TPP	S1-C2-N3	2.30	115.21	112.30
5	A	1236	TPP	C7'-N3-C2	-2.24	118.81	123.48
5	B	1236	TPP	O3A-PB-O1B	-2.21	99.43	111.04

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1236	TPP	C5'-C7'-N3-C2
5	B	1236	TPP	C5-C6-C7-O7
5	B	1236	TPP	C7-O7-PA-O1A
5	A	1236	TPP	C5'-C7'-N3-C4
5	A	1236	TPP	S1-C5-C6-C7
5	B	1236	TPP	S1-C5-C6-C7
5	A	1236	TPP	C5-C6-C7-O7
5	A	1236	TPP	C4-C5-C6-C7
5	B	1236	TPP	C5'-C7'-N3-C2
5	A	1236	TPP	C7-O7-PA-O1A
5	B	1236	TPP	C7-O7-PA-O3A
5	B	1236	TPP	C4-C5-C6-C7
5	B	1236	TPP	C5'-C7'-N3-C4
5	A	1236	TPP	PA-O3A-PB-O2B
5	B	1236	TPP	PA-O3A-PB-O2B

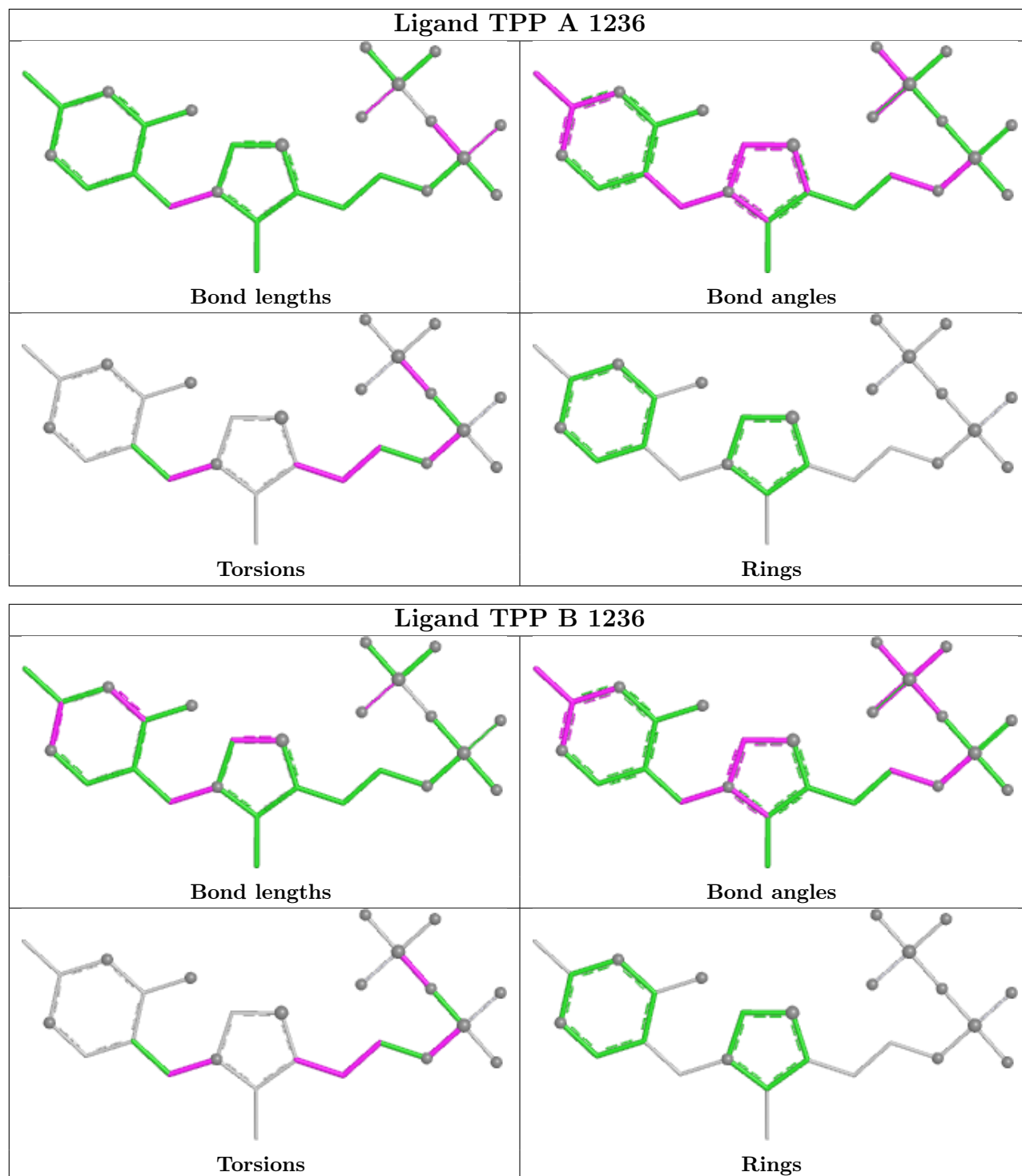
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1233	SF4	1	0
5	A	1236	TPP	1	0
5	B	1236	TPP	1	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

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.