



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:13 PM EDT

PDB ID : 1KEK / pdb_00001kek
Title : Crystal Structure of the Free Radical Intermediate of Pyruvate:Ferredoxin Oxidoreductase
Authors : Chabriere, E.; Vernede, X.; Guigliarelli, B.; Charon, M.-H.; Hatchikian, E.C.; Fontecilla-Camps, J.C.
Deposited on : 2001-11-16
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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)	:	2.50

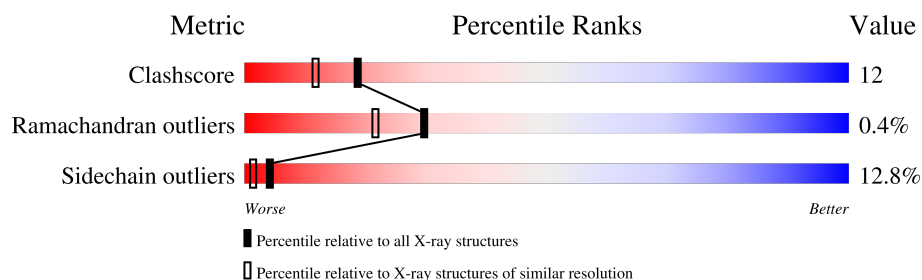
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 67% 25% 5% •
1	B	1231	 69% 23% 6% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20775 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate-Ferredoxin Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	36	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	41	0	0
			9383	5941	1599	1784	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).

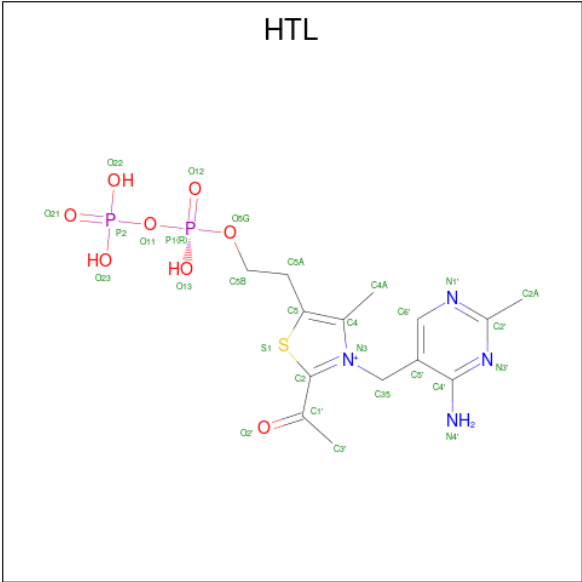
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

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



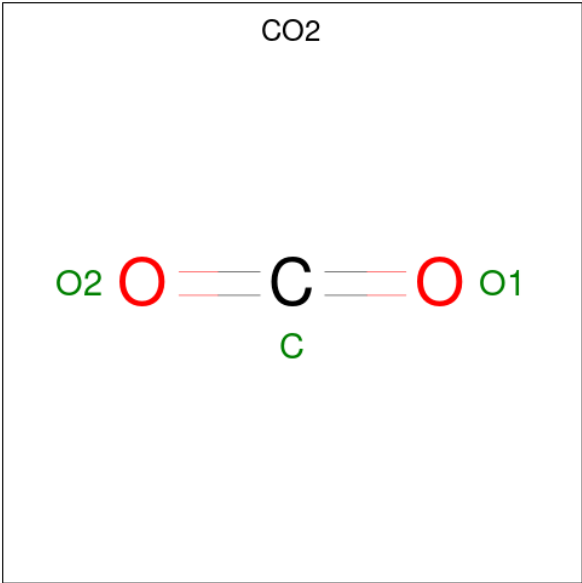
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-ACETYL-THIAMINE DIPHOSPHATE (CCD ID: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		

- Molecule 6 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			3	1 2		
6	B	1	Total	C O	0	0
			3	1 2		

- Molecule 7 is water.

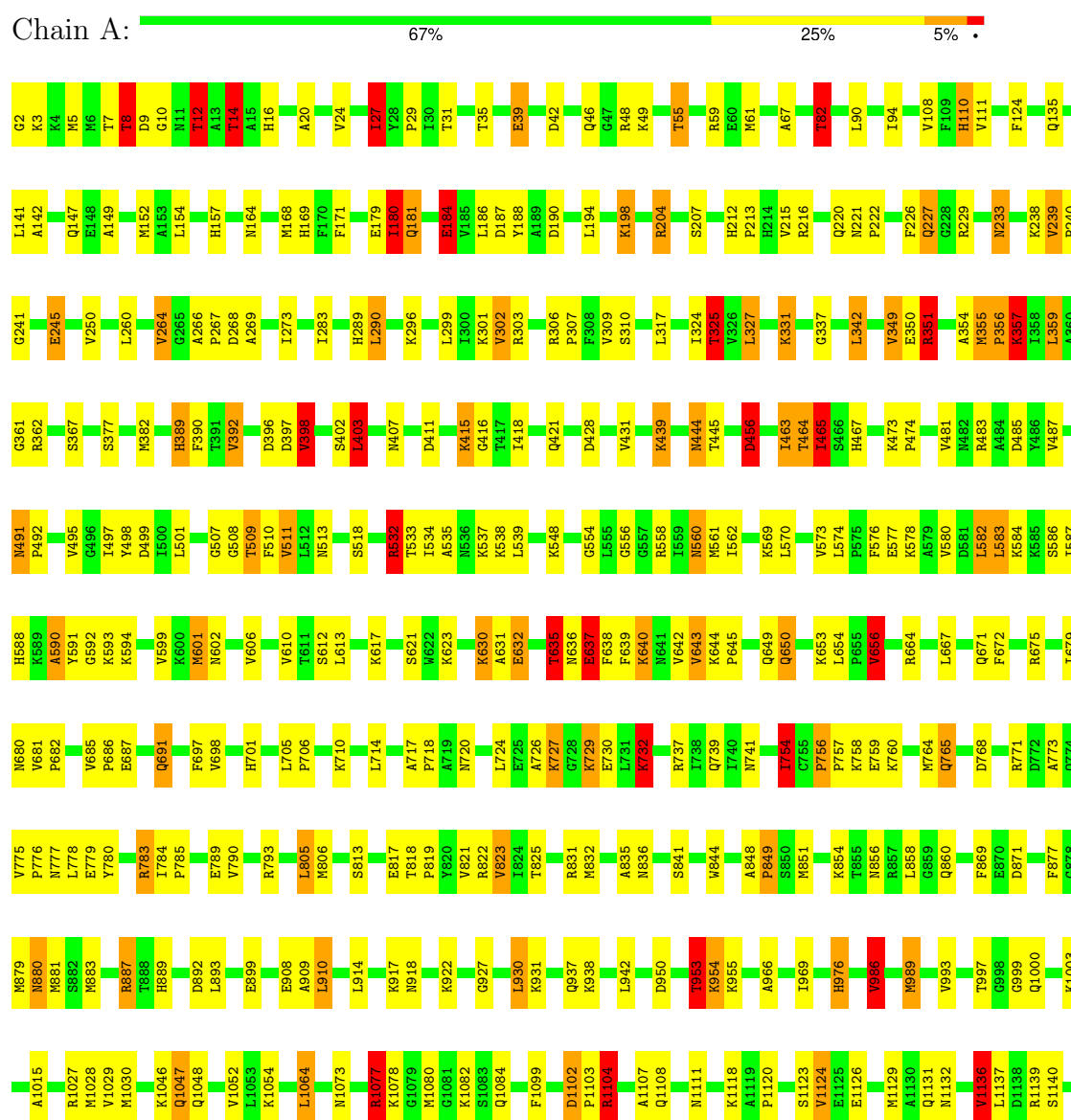
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	851	Total 851	O 851	0	0
7	B	1042	Total 1042	O 1042	0	0

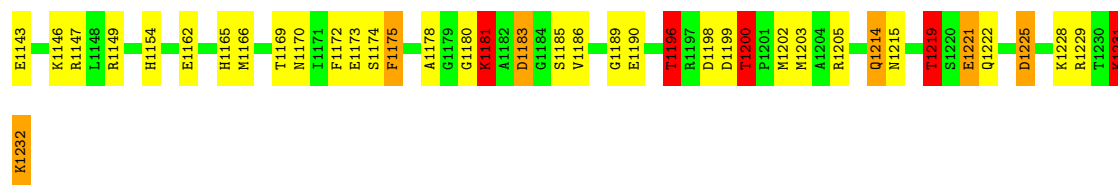
3 Residue-property plots

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.

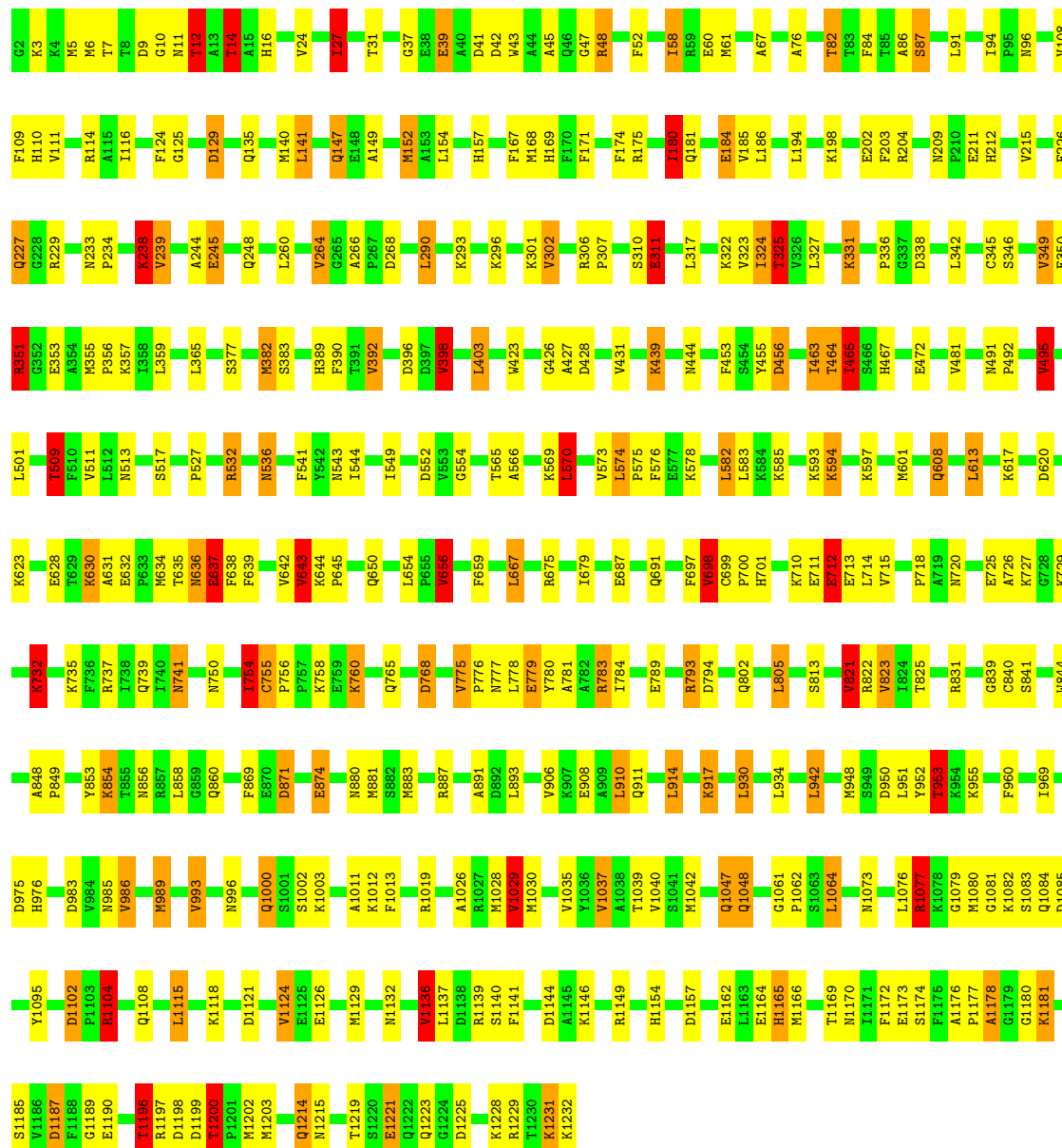
• Molecule 1: Pyruvate-Ferredoxin Oxidoreductase





• Molecule 1: Pyruvate-Ferredoxin Oxidoreductase

Chain B: 69% 23% 6%



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	86.11Å 145.76Å 210.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.38 – 1.90	Depositor
% Data completeness (in resolution range)	97.5 (27.38-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR, REFMAC	Depositor
R, R_{free}	0.178 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20775	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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, HTL, SF4, MG, CO2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	12/9585 (0.1%)	1.89	213/12954 (1.6%)
1	B	1.32	17/9585 (0.2%)	1.94	228/12954 (1.8%)
All	All	1.19	29/19170 (0.2%)	1.91	441/25908 (1.7%)

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	2
1	B	2	3
All	All	2	5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1231	LYS	C-N	47.86	2.00	1.33
1	B	732	LYS	CD-CE	47.06	2.93	1.52
1	A	601	MET	CA-C	27.25	1.89	1.52
1	A	601	MET	C-O	-25.39	0.94	1.24
1	B	711	GLU	C-O	-24.81	0.94	1.24
1	A	532	ARG	CA-C	24.32	1.83	1.52
1	B	732	LYS	CG-CD	-23.11	0.83	1.52
1	B	712	GLU	C-O	-21.45	0.97	1.24
1	B	712	GLU	CA-C	19.82	1.79	1.52
1	A	601	MET	CA-CB	-19.32	1.22	1.53
1	B	711	GLU	CA-CB	-17.12	1.26	1.53
1	B	1126	GLU	C-O	-15.47	1.06	1.24
1	B	732	LYS	CA-CB	-13.99	1.29	1.53
1	B	711	GLU	CA-C	13.67	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	712	GLU	CA-CB	-11.92	1.33	1.53
1	A	532	ARG	CA-CB	-10.60	1.36	1.53
1	A	532	ARG	C-N	-9.32	1.21	1.33
1	B	245	GLU	C-O	-9.28	1.13	1.24
1	A	637	GLU	CA-C	9.14	1.65	1.52
1	B	48	ARG	CD-NE	-8.98	1.33	1.46
1	A	1147	ARG	CG-CD	7.78	1.75	1.52
1	A	637	GLU	CA-CB	7.68	1.66	1.53
1	A	637	GLU	C-N	-7.37	1.23	1.33
1	B	636	ASN	CA-CB	5.96	1.63	1.53
1	A	908	GLU	CB-CG	-5.88	1.34	1.52
1	A	48	ARG	CD-NE	-5.68	1.38	1.46
1	B	839	GLY	N-CA	5.62	1.50	1.45
1	B	1126	GLU	CA-CB	-5.50	1.44	1.53
1	B	456	ASP	CA-CB	5.33	1.62	1.53

All (441) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	ARG	CD-NE-CZ	34.98	173.37	124.40
1	B	48	ARG	CD-NE-CZ	29.70	165.97	124.40
1	A	204	ARG	CD-NE-CZ	29.41	165.58	124.40
1	A	601	MET	O-C-N	29.23	153.10	122.12
1	B	732	LYS	CG-CD-CE	-26.21	51.01	111.30
1	A	532	ARG	O-C-N	18.28	140.90	122.07
1	B	732	LYS	N-CA-CB	18.20	141.25	110.49
1	A	1200	THR	N-CA-CB	-17.75	89.49	109.72
1	A	532	ARG	CA-C-O	-16.90	103.08	120.82
1	A	601	MET	N-CA-CB	16.62	135.00	110.06
1	B	712	GLU	N-CA-CB	16.23	135.22	110.22
1	B	712	GLU	O-C-N	14.98	139.75	122.22
1	A	239	VAL	N-CA-CB	14.89	119.88	110.50
1	B	239	VAL	N-CA-CB	14.13	119.40	110.50
1	A	48	ARG	CD-NE-CZ	14.01	144.01	124.40
1	B	48	ARG	CG-CD-NE	13.94	142.67	112.00
1	A	306	ARG	CA-C-O	-13.42	107.51	119.72
1	A	1124	VAL	CB-CA-C	-12.94	95.32	111.88
1	A	1136	VAL	CB-CA-C	-12.83	94.82	112.14
1	A	848	ALA	CA-C-O	-12.43	107.25	120.17
1	B	1200	THR	N-CA-CB	-12.25	95.75	109.72
1	B	636	ASN	CA-CB-CG	-12.18	100.42	112.60
1	B	1073	ASN	CA-CB-CG	11.75	124.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1124	VAL	N-CA-CB	11.71	123.51	110.51
1	A	637	GLU	N-CA-C	-11.41	98.74	112.89
1	B	711	GLU	O-C-N	11.39	135.21	122.11
1	A	1219	THR	N-CA-CB	-11.07	94.53	110.36
1	A	1196	THR	N-CA-CB	-11.00	94.41	110.80
1	A	31	THR	CA-C-O	-11.00	108.37	120.25
1	B	1136	VAL	CB-CA-C	-10.97	94.48	112.26
1	B	775	VAL	CA-C-O	10.72	125.88	118.69
1	A	48	ARG	NE-CZ-NH2	-10.66	109.60	119.20
1	A	27	ILE	CA-CB-CG2	10.63	128.57	110.50
1	B	711	GLU	N-CA-CB	10.58	127.03	109.78
1	B	985	ASN	OD1-CG-ND2	10.48	133.08	122.60
1	B	1141	PHE	CA-CB-CG	10.44	124.24	113.80
1	A	216	ARG	CD-NE-CZ	10.32	138.85	124.40
1	B	1104	ARG	CD-NE-CZ	10.22	138.71	124.40
1	A	532	ARG	CA-C-N	-9.78	106.40	120.29
1	A	532	ARG	C-N-CA	-9.78	106.40	120.29
1	A	356	PRO	CA-C-O	-9.72	114.12	121.31
1	B	1126	GLU	N-CA-CB	9.72	124.40	110.12
1	A	351	ARG	CD-NE-CZ	9.70	137.98	124.40
1	B	27	ILE	CA-CB-CG2	9.58	126.78	110.50
1	B	27	ILE	N-CA-CB	-9.56	96.41	112.47
1	B	1196	THR	N-CA-CB	-9.55	96.58	110.80
1	B	355	MET	CA-CB-CG	9.49	133.09	114.10
1	B	31	THR	CA-C-O	-9.45	110.34	120.17
1	B	48	ARG	NH1-CZ-NH2	9.42	131.55	119.30
1	B	82	THR	CB-CA-C	-9.40	89.71	110.67
1	A	601	MET	CA-C-O	-9.37	110.51	120.63
1	A	351	ARG	NE-CZ-NH1	9.35	130.85	121.50
1	B	1124	VAL	CB-CA-C	-9.32	99.83	112.04
1	B	1124	VAL	N-CA-CB	9.31	122.11	110.47
1	B	392	VAL	CB-CA-C	-9.24	95.68	110.28
1	B	456	ASP	CA-CB-CG	-9.23	103.37	112.60
1	A	908	GLU	CA-CB-CG	9.22	132.55	114.10
1	A	306	ARG	O-C-N	9.20	132.64	121.79
1	B	465	ILE	CB-CA-C	9.16	123.78	110.77
1	A	1136	VAL	N-CA-CB	9.10	122.92	110.54
1	A	1104	ARG	CD-NE-CZ	9.04	137.05	124.40
1	B	428	ASP	CA-CB-CG	8.97	121.57	112.60
1	B	1165	HIS	N-CA-CB	8.93	124.12	110.28
1	A	204	ARG	NE-CZ-NH1	-8.91	112.59	121.50
1	B	637	GLU	CB-CG-CD	8.89	127.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	821	VAL	N-CA-CB	8.87	123.88	110.58
1	B	1221	GLU	CA-CB-CG	8.64	131.38	114.10
1	A	180	ILE	CA-CB-CG2	8.63	125.17	110.50
1	A	532	ARG	N-CA-CB	8.63	122.52	110.01
1	A	27	ILE	N-CA-CB	-8.63	97.98	112.47
1	A	1165	HIS	N-CA-CB	8.59	123.59	110.28
1	A	351	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	A	601	MET	CA-C-N	-8.44	106.15	120.58
1	A	601	MET	C-N-CA	-8.44	106.15	120.58
1	B	1164	GLU	CA-C-O	-8.44	111.96	120.82
1	A	880	ASN	CA-CB-CG	8.43	121.03	112.60
1	B	392	VAL	N-CA-CB	8.40	125.19	111.58
1	A	832	MET	CA-CB-CG	8.37	130.84	114.10
1	A	465	ILE	CB-CA-C	8.36	121.71	110.42
1	A	637	GLU	CA-C-O	-8.36	108.94	119.31
1	A	392	VAL	CB-CA-C	-8.34	97.10	110.28
1	B	993	VAL	N-CA-CB	-8.33	98.84	109.84
1	A	756	PRO	N-CA-C	8.24	120.75	110.70
1	A	1225	ASP	CA-CB-CG	8.21	120.81	112.60
1	B	1047	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	A	675	ARG	CD-NE-CZ	8.09	135.72	124.40
1	B	1013	PHE	CA-CB-CG	-8.04	105.75	113.80
1	A	8	THR	N-CA-CB	8.03	124.62	111.21
1	B	732	LYS	CB-CA-C	-8.01	94.49	110.42
1	B	1136	VAL	N-CA-CB	8.00	125.25	110.77
1	A	82	THR	CB-CA-C	-7.99	92.85	110.67
1	B	264	VAL	N-CA-CB	-7.96	98.39	111.44
1	A	238	LYS	CA-C-N	-7.92	115.25	120.24
1	A	238	LYS	C-N-CA	-7.92	115.25	120.24
1	A	389	HIS	CA-CB-CG	-7.89	105.91	113.80
1	A	428	ASP	CA-CB-CG	7.83	120.43	112.60
1	B	245	GLU	O-C-N	-7.79	114.04	122.07
1	B	238	LYS	CA-C-N	-7.73	115.37	120.24
1	B	238	LYS	C-N-CA	-7.73	115.37	120.24
1	A	39	GLU	CA-CB-CG	-7.68	98.75	114.10
1	A	679	ILE	N-CA-C	-7.68	104.31	111.45
1	A	1104	ARG	NE-CZ-NH2	7.66	126.09	119.20
1	A	48	ARG	NH1-CZ-NH2	7.64	129.23	119.30
1	A	848	ALA	O-C-N	7.61	129.14	121.30
1	B	325	THR	N-CA-CB	7.58	123.41	110.68
1	B	712	GLU	CA-C-N	-7.56	108.70	122.38
1	B	712	GLU	C-N-CA	-7.56	108.70	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	756	PRO	N-CA-C	7.56	119.92	110.70
1	B	953	THR	CA-CB-OG1	7.54	120.90	109.60
1	B	306	ARG	CA-C-O	-7.50	111.92	120.03
1	B	871	ASP	N-CA-C	7.46	121.69	112.59
1	B	109	PHE	CA-CB-CG	7.45	121.25	113.80
1	A	889	HIS	CA-CB-CG	7.43	121.23	113.80
1	B	1047	GLN	CB-CG-CD	7.41	125.19	112.60
1	B	125	GLY	N-CA-C	7.40	124.17	111.15
1	A	331	LYS	CA-CB-CG	7.35	128.80	114.10
1	B	698	VAL	N-CA-CB	-7.31	94.92	111.87
1	B	659	PHE	CA-CB-CG	-7.30	106.50	113.80
1	B	42	ASP	CA-CB-CG	7.27	119.87	112.60
1	B	675	ARG	CD-NE-CZ	7.26	134.57	124.40
1	A	349	VAL	N-CA-CB	7.26	121.47	110.58
1	B	264	VAL	CB-CA-C	7.26	121.68	110.50
1	A	1104	ARG	CG-CD-NE	-7.23	96.09	112.00
1	A	1205	ARG	NE-CZ-NH1	-7.21	114.29	121.50
1	B	1172	PHE	CA-C-O	7.21	129.42	121.06
1	B	465	ILE	CA-CB-CG2	7.20	122.74	110.50
1	A	110	HIS	CA-CB-CG	-7.17	106.63	113.80
1	A	1183	ASP	N-CA-C	7.17	120.71	109.96
1	B	349	VAL	N-CA-CB	7.16	121.32	110.58
1	B	701	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	398	VAL	CB-CA-C	7.13	119.75	111.55
1	B	1121	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	953	THR	CA-CB-OG1	7.09	120.23	109.60
1	B	911	GLN	CB-CG-CD	7.09	124.65	112.60
1	A	887	ARG	NE-CZ-NH2	7.08	125.57	119.20
1	B	1011	ALA	CA-C-O	-7.07	113.89	121.38
1	B	453	PHE	CA-CB-CG	-7.07	106.73	113.80
1	B	822	ARG	NE-CZ-NH1	-7.07	114.43	121.50
1	A	650	GLN	OE1-CD-NE2	7.05	129.66	122.60
1	B	147	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	754	ILE	CA-CB-CG2	7.04	122.46	110.50
1	B	1077	ARG	NE-CZ-NH2	-7.03	112.88	119.20
1	B	985	ASN	CA-C-N	-7.01	114.49	123.19
1	B	985	ASN	C-N-CA	-7.01	114.49	123.19
1	A	637	GLU	CA-CB-CG	6.96	128.02	114.10
1	B	174	PHE	CA-CB-CG	-6.96	106.84	113.80
1	A	337	GLY	CA-C-O	-6.90	114.86	121.62
1	A	180	ILE	CB-CA-C	6.89	120.69	110.98
1	B	755	CYS	CA-C-O	-6.88	113.60	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ILE	CA-CB-CG2	6.86	122.16	110.50
1	B	697	PHE	CA-CB-CG	6.79	120.59	113.80
1	A	1104	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	B	14	THR	CA-CB-OG1	6.78	119.77	109.60
1	A	877	PHE	CA-C-O	6.78	127.73	120.55
1	A	986	VAL	N-CA-CB	6.76	120.45	111.25
1	B	302	VAL	N-CA-CB	6.72	118.05	110.72
1	A	592	GLY	N-CA-C	-6.71	105.96	115.43
1	B	96	ASN	CA-CB-CG	-6.71	105.89	112.60
1	B	1104	ARG	CG-CD-NE	-6.69	97.28	112.00
1	B	608	GLN	CB-CG-CD	6.66	123.92	112.60
1	A	356	PRO	CB-CA-C	-6.64	102.54	112.04
1	A	407	ASN	CA-CB-CG	-6.64	105.96	112.60
1	B	911	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	B	1085	ASP	CA-CB-CG	-6.62	105.98	112.60
1	B	552	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	456	ASP	CA-CB-CG	-6.60	106.00	112.60
1	B	48	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	A	55	THR	OG1-CB-CG2	-6.59	96.12	109.30
1	A	456	ASP	CA-C-O	-6.59	114.22	121.87
1	A	264	VAL	N-CA-CB	-6.59	99.60	111.92
1	A	1205	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	B	754	ILE	CA-CB-CG2	6.57	121.67	110.50
1	B	245	GLU	CA-C-N	6.57	129.74	120.28
1	B	245	GLU	C-N-CA	6.57	129.74	120.28
1	A	976	HIS	CA-CB-CG	-6.54	107.26	113.80
1	B	1196	THR	CB-CA-C	6.49	121.27	109.99
1	A	922	LYS	CG-CD-CE	6.46	126.15	111.30
1	B	794	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	226	PHE	CA-CB-CG	6.41	120.20	113.80
1	B	307	PRO	N-CA-CB	6.37	109.61	102.60
1	B	204	ARG	N-CA-CB	6.36	119.23	110.01
1	B	48	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	A	82	THR	CA-CB-OG1	6.33	119.10	109.60
1	A	233	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	532	ARG	CB-CA-C	-6.32	100.96	110.88
1	B	464	THR	CA-C-N	-6.32	114.70	123.10
1	B	464	THR	C-N-CA	-6.32	114.70	123.10
1	B	1037	VAL	O-C-N	-6.31	116.35	123.10
1	B	732	LYS	N-CA-C	6.29	124.20	110.80
1	A	264	VAL	CA-CB-CG1	6.29	121.08	110.40
1	B	793	ARG	N-CA-CB	-6.27	100.56	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ILE	CA-CB-CG2	6.25	121.13	110.50
1	A	1165	HIS	CA-CB-CG	-6.24	107.56	113.80
1	B	96	ASN	OD1-CG-ND2	6.23	128.83	122.60
1	A	499	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	760	LYS	N-CA-C	6.22	119.02	110.24
1	A	48	ARG	CB-CG-CD	-6.22	97.00	111.30
1	B	541	PHE	CA-CB-CG	6.22	120.02	113.80
1	B	741	ASN	CA-CB-CG	6.21	118.81	112.60
1	B	755	CYS	O-C-N	6.19	126.30	121.47
1	A	1219	THR	OG1-CB-CG2	6.18	121.67	109.30
1	B	822	ARG	NE-CZ-NH2	6.18	124.77	119.20
1	B	989	MET	CG-SD-CE	-6.17	87.33	100.90
1	B	39	GLU	CA-CB-CG	-6.12	101.85	114.10
1	A	592	GLY	CA-C-O	6.12	126.10	119.06
1	A	664	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	A	14	THR	CA-CB-OG1	6.10	118.75	109.60
1	A	184	GLU	CA-CB-CG	6.10	126.30	114.10
1	B	1126	GLU	CA-C-O	6.08	126.99	120.55
1	A	190	ASP	CA-C-O	6.07	126.85	120.42
1	B	456	ASP	N-CA-C	6.02	118.68	110.55
1	A	485	ASP	CA-C-O	6.02	126.64	119.60
1	A	39	GLU	CG-CD-OE2	-6.02	104.56	118.40
1	B	351	ARG	NE-CZ-NH1	6.02	127.52	121.50
1	A	302	VAL	CA-CB-CG2	6.01	120.61	110.40
1	A	910	LEU	CA-C-O	6.00	126.91	120.55
1	B	325	THR	CA-CB-OG1	6.00	118.59	109.60
1	B	960	PHE	CA-CB-CG	5.99	119.79	113.80
1	B	82	THR	N-CA-CB	5.98	121.30	111.62
1	B	444	ASN	CB-CG-ND2	5.97	125.36	116.40
1	B	821	VAL	CA-C-O	-5.97	114.52	120.85
1	A	403	LEU	N-CA-CB	-5.95	102.26	110.29
1	B	1095	TYR	O-C-N	5.95	128.43	122.12
1	B	608	GLN	CA-CB-CG	5.95	125.99	114.10
1	A	1052	VAL	O-C-N	5.94	127.63	121.87
1	A	207	SER	CA-CB-OG	-5.92	99.27	111.10
1	B	823	VAL	CA-CB-CG2	5.91	120.45	110.40
1	A	701	HIS	CA-CB-CG	-5.91	107.89	113.80
1	B	306	ARG	NE-CZ-NH1	5.91	127.41	121.50
1	A	164	ASN	CA-C-N	-5.90	117.61	123.04
1	A	164	ASN	C-N-CA	-5.90	117.61	123.04
1	A	220	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	A	656	VAL	CA-CB-CG2	5.88	120.40	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	PHE	CA-CB-CG	-5.88	107.92	113.80
1	B	1214	GLN	N-CA-CB	-5.87	102.46	110.56
1	A	835	ALA	CA-C-O	-5.86	114.51	120.84
1	A	8	THR	CB-CA-C	-5.85	98.03	111.95
1	A	82	THR	N-CA-CB	5.85	121.10	111.62
1	A	415	LYS	CA-C-N	-5.84	116.49	123.44
1	A	415	LYS	C-N-CA	-5.84	116.49	123.44
1	B	1077	ARG	N-CA-C	5.84	118.42	111.71
1	B	58	ILE	CB-CA-C	-5.82	101.83	110.33
1	B	1029	VAL	CA-CB-CG2	5.81	120.27	110.40
1	A	42	ASP	N-CA-CB	5.80	118.42	110.01
1	B	634	MET	N-CA-CB	5.80	118.94	109.95
1	B	1214	GLN	OE1-CD-NE2	5.80	128.40	122.60
1	A	1172	PHE	CA-C-O	5.78	127.53	120.60
1	A	637	GLU	N-CA-CB	-5.77	101.00	110.40
1	B	712	GLU	CA-C-O	-5.75	113.60	120.10
1	A	356	PRO	N-CA-C	5.75	123.83	113.70
1	A	1196	THR	CB-CA-C	5.75	119.99	109.99
1	A	14	THR	N-CA-CB	5.74	119.14	110.30
1	A	94	ILE	O-C-N	-5.74	116.75	120.42
1	A	851	MET	CA-C-N	5.73	127.00	119.84
1	A	851	MET	C-N-CA	5.73	127.00	119.84
1	B	643	VAL	N-CA-CB	5.72	117.90	110.57
1	A	110	HIS	CA-C-N	-5.71	115.18	123.06
1	A	110	HIS	C-N-CA	-5.71	115.18	123.06
1	B	536	ASN	CA-C-O	-5.71	114.50	120.55
1	B	517	SER	N-CA-C	5.71	117.58	111.36
1	A	310	SER	CA-CB-OG	-5.70	99.70	111.10
1	A	823	VAL	CA-CB-CG2	5.70	120.09	110.40
1	B	821	VAL	O-C-N	5.70	127.70	121.83
1	A	1221	GLU	CA-CB-CG	5.68	125.45	114.10
1	B	543	ASN	CA-CB-CG	-5.67	106.93	112.60
1	B	643	VAL	CA-C-O	-5.67	114.75	121.05
1	A	464	THR	CA-C-N	-5.67	114.93	122.98
1	A	464	THR	C-N-CA	-5.67	114.93	122.98
1	B	82	THR	OG1-CB-CG2	5.67	120.64	109.30
1	B	324	ILE	CA-CB-CG2	5.67	120.13	110.50
1	A	1077	ARG	N-CA-C	5.67	118.22	111.71
1	B	509	THR	N-CA-CB	5.66	119.46	110.57
1	A	402	SER	CA-C-O	5.64	127.95	121.47
1	B	1200	THR	CA-CB-CG2	5.64	120.08	110.50
1	A	491	ASN	OD1-CG-ND2	-5.63	116.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	SER	CA-CB-OG	-5.63	99.85	111.10
1	B	679	ILE	N-CA-C	-5.61	106.23	111.45
1	B	392	VAL	CA-C-O	-5.59	114.33	120.43
1	B	983	ASP	CA-C-O	5.59	128.20	121.66
1	B	975	ASP	N-CA-CB	-5.59	101.91	110.12
1	B	853	TYR	CA-C-O	-5.58	114.91	121.16
1	B	1157	ASP	CA-C-N	5.58	127.71	120.56
1	B	1157	ASP	C-N-CA	5.58	127.71	120.56
1	A	1108	GLN	CA-CB-CG	5.58	125.26	114.10
1	A	1200	THR	O-C-N	-5.58	115.69	120.99
1	B	1061	GLY	N-CA-C	-5.57	100.97	112.34
1	A	511	VAL	N-CA-CB	5.57	118.82	111.25
1	A	12	THR	CA-CB-OG1	5.56	117.93	109.60
1	A	46	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	B	848	ALA	CA-C-O	-5.55	114.53	119.75
1	A	590	ALA	N-CA-C	-5.55	102.31	110.52
1	A	793	ARG	CG-CD-NE	-5.54	99.81	112.00
1	A	836	ASN	CA-C-O	-5.53	114.40	120.43
1	A	1102	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	444	ASN	CA-CB-CG	-5.52	107.08	112.60
1	B	1102	ASP	CA-C-N	5.52	125.35	119.28
1	B	1102	ASP	C-N-CA	5.52	125.35	119.28
1	A	269	ALA	O-C-N	5.52	129.66	122.87
1	B	1073	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	954	LYS	CA-CB-CG	-5.51	103.08	114.10
1	B	244	ALA	O-C-N	5.50	127.95	122.12
1	B	760	LYS	N-CA-C	5.50	118.21	110.23
1	B	631	ALA	N-CA-C	-5.50	105.24	112.72
1	A	290	LEU	N-CA-C	5.49	117.35	111.36
1	B	311	GLU	CA-CB-CG	5.49	125.08	114.10
1	A	456	ASP	CB-CA-C	-5.49	98.44	109.68
1	A	226	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	899	GLU	CA-CB-CG	5.48	125.06	114.10
1	B	456	ASP	CB-CA-C	-5.48	98.85	109.76
1	B	1002	SER	CA-C-O	-5.48	115.22	121.58
1	B	636	ASN	CA-C-O	-5.48	115.26	121.72
1	A	649	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	B	1214	GLN	N-CA-C	5.47	119.06	112.93
1	B	76	ALA	O-C-N	5.46	128.61	122.22
1	B	1081	GLY	N-CA-C	-5.45	108.67	114.67
1	A	29	PRO	CB-CA-C	-5.45	104.73	111.11
1	A	269	ALA	CA-C-O	-5.45	115.20	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	871	ASP	N-CA-CB	-5.44	102.21	110.92
1	B	114	ARG	CA-C-N	5.44	128.57	120.90
1	B	114	ARG	C-N-CA	5.44	128.57	120.90
1	A	793	ARG	N-CA-CB	-5.43	101.85	110.22
1	B	306	ARG	O-C-N	5.43	127.64	121.94
1	B	377	SER	CA-CB-OG	-5.43	100.23	111.10
1	B	86	ALA	CB-CA-C	-5.42	100.70	110.03
1	A	245	GLU	CA-CB-CG	5.41	124.92	114.10
1	A	392	VAL	CA-C-O	-5.41	114.54	120.43
1	A	325	THR	CA-CB-OG1	5.40	117.70	109.60
1	B	302	VAL	CB-CA-C	5.40	117.61	110.91
1	B	735	LYS	CA-C-O	-5.40	114.98	120.71
1	A	361	GLY	O-C-N	5.40	128.17	123.36
1	A	1175	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	1120	PRO	CA-C-O	-5.39	115.45	121.32
1	B	382	MET	CA-C-N	-5.38	113.66	122.54
1	B	382	MET	C-N-CA	-5.38	113.66	122.54
1	A	1077	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	685	VAL	CA-C-N	5.36	125.69	119.47
1	A	685	VAL	C-N-CA	5.36	125.69	119.47
1	B	338	ASP	CB-CA-C	5.35	119.14	109.45
1	B	565	THR	CA-C-O	-5.35	114.88	120.55
1	B	754	ILE	N-CA-CB	-5.34	100.43	111.76
1	B	301	LYS	CA-C-N	-5.32	115.50	122.37
1	B	301	LYS	C-N-CA	-5.32	115.50	122.37
1	B	983	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	966	ALA	N-CA-C	5.32	117.99	111.82
1	A	1027	ARG	CD-NE-CZ	5.32	131.84	124.40
1	B	642	VAL	CA-C-N	-5.32	113.76	120.56
1	B	642	VAL	C-N-CA	-5.32	113.76	120.56
1	B	636	ASN	CB-CG-ND2	5.31	124.37	116.40
1	B	1039	THR	CA-C-O	-5.31	114.97	120.70
1	B	12	THR	CA-C-O	-5.30	113.54	119.79
1	A	245	GLU	CB-CG-CD	5.29	121.60	112.60
1	A	1147	ARG	CG-CD-NE	-5.29	100.37	112.00
1	A	698	VAL	N-CA-CB	-5.28	99.77	111.50
1	A	691	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	B	167	PHE	CA-C-O	5.25	127.05	121.11
1	B	398	VAL	N-CA-CB	5.24	120.04	110.86
1	B	793	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	A	999	GLY	CA-C-O	-5.23	113.77	119.88
1	B	712	GLU	N-CA-C	5.23	117.72	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ALA	O-C-N	5.22	129.30	123.19
1	A	325	THR	N-CA-CB	5.22	119.46	110.68
1	A	771	ARG	N-CA-C	5.22	116.66	111.07
1	B	715	VAL	N-CA-C	5.22	115.66	110.23
1	B	754	ILE	CA-CB-CG1	-5.21	101.54	110.40
1	A	986	VAL	CA-C-N	-5.21	115.65	123.00
1	A	986	VAL	C-N-CA	-5.21	115.65	123.00
1	B	1144	ASP	O-C-N	5.21	128.09	122.15
1	B	336	PRO	N-CA-C	-5.21	107.62	114.03
1	A	1047	GLN	CB-CG-CD	5.20	121.44	112.60
1	B	464	THR	CA-C-O	-5.20	115.09	120.70
1	A	357	LYS	CA-C-N	-5.19	116.19	123.10
1	A	357	LYS	C-N-CA	-5.19	116.19	123.10
1	B	1115	LEU	CA-C-O	-5.19	114.61	120.43
1	B	209	ASN	CA-CB-CG	-5.19	107.41	112.60
1	B	331	LYS	CD-CE-NZ	-5.19	95.30	111.90
1	B	290	LEU	CA-C-N	5.18	127.23	120.28
1	B	290	LEU	C-N-CA	5.18	127.23	120.28
1	A	1196	THR	CA-CB-OG1	5.18	117.37	109.60
1	A	1221	GLU	CB-CG-CD	5.18	121.41	112.60
1	B	87	SER	N-CA-C	5.18	116.18	108.31
1	A	986	VAL	CA-CB-CG1	5.17	119.19	110.40
1	A	1175	PHE	CA-C-O	5.17	126.61	120.66
1	B	124	PHE	N-CA-C	5.17	118.08	110.59
1	B	650	GLN	OE1-CD-NE2	5.17	127.77	122.60
1	A	301	LYS	CA-C-N	-5.17	116.29	122.90
1	A	301	LYS	C-N-CA	-5.17	116.29	122.90
1	A	635	THR	CB-CA-C	5.17	120.70	110.42
1	A	351	ARG	CG-CD-NE	5.17	123.36	112.00
1	A	307	PRO	N-CA-CB	5.15	108.27	102.60
1	B	1082	LYS	CG-CD-CE	5.15	123.15	111.30
1	A	31	THR	O-C-N	5.15	127.20	121.43
1	B	565	THR	O-C-N	5.15	127.58	122.12
1	A	680	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	B	952	TYR	CA-C-N	-5.14	114.06	121.42
1	B	952	TYR	C-N-CA	-5.14	114.06	121.42
1	A	664	ARG	NH1-CZ-NH2	5.14	125.98	119.30
1	B	455	TYR	CA-C-O	-5.13	115.62	121.68
1	A	741	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	495	VAL	N-CA-CB	-5.13	101.88	110.65
1	A	1073	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	914	LEU	O-C-N	5.13	127.56	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1214	GLN	N-CA-CB	-5.13	103.48	110.56
1	B	47	GLY	O-C-N	-5.12	116.46	122.45
1	B	94	ILE	N-CA-C	5.11	119.06	112.67
1	B	570	LEU	N-CA-C	5.11	120.37	113.72
1	A	241	GLY	CA-C-N	5.11	127.10	120.56
1	A	241	GLY	C-N-CA	5.11	127.10	120.56
1	B	209	ASN	CA-C-N	5.11	124.83	119.82
1	B	209	ASN	C-N-CA	5.11	124.83	119.82
1	B	398	VAL	CB-CA-C	5.11	117.42	111.55
1	B	323	VAL	O-C-N	5.11	128.72	123.05
1	B	266	ALA	CA-C-N	5.10	124.77	119.56
1	B	266	ALA	C-N-CA	5.10	124.77	119.56
1	A	213	PRO	O-C-N	5.10	129.36	123.14
1	B	667	LEU	CA-C-N	5.10	130.90	120.80
1	B	667	LEU	C-N-CA	5.10	130.90	120.80
1	A	415	LYS	CA-C-O	-5.10	115.11	120.92
1	A	908	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	1103	PRO	CA-C-N	-5.09	112.22	120.72
1	A	1103	PRO	C-N-CA	-5.09	112.22	120.72
1	B	152	MET	CG-SD-CE	-5.09	89.70	100.90
1	A	397	ASP	CA-C-N	-5.08	116.35	122.35
1	A	397	ASP	C-N-CA	-5.08	116.35	122.35
1	A	1073	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	768	ASP	CA-CB-CG	-5.08	107.52	112.60
1	B	175	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	392	VAL	O-C-N	5.06	128.53	123.07
1	A	1131	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	345	CYS	CA-C-O	-5.06	115.19	120.55
1	A	1214	GLN	CG-CD-NE2	-5.05	108.82	116.40
1	A	508	GLY	CA-C-O	-5.05	115.40	122.51
1	B	60	GLU	CA-C-O	-5.04	114.85	120.54
1	A	82	THR	OG1-CB-CG2	5.04	119.37	109.30
1	B	1187	ASP	CA-CB-CG	-5.02	107.58	112.60
1	B	656	VAL	CA-CB-CG1	5.02	118.94	110.40
1	B	203	PHE	O-C-N	-5.02	116.80	122.12
1	B	821	VAL	CA-CB-CG2	5.01	118.92	110.40
1	A	239	VAL	CB-CA-C	-5.01	109.04	114.35
1	B	793	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	B	307	PRO	CA-N-CD	-5.01	104.49	111.50
1	A	879	MET	O-C-N	5.00	127.42	122.12

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	712	GLU	CA
1	B	732	LYS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	ARG	Mainchain
1	A	637	GLU	Mainchain
1	B	1029	VAL	Mainchain
1	B	129	ASP	Mainchain
1	B	712	GLU	Mainchain

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	9383	0	9263	256	0
1	B	9383	0	9261	216	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	0	0
4	B	24	0	0	0	0
5	A	29	0	18	3	0
5	B	29	0	18	2	0
6	A	3	0	0	1	0
6	B	3	0	0	1	0
7	A	851	0	0	36	0
7	B	1042	0	0	31	0
All	All	20775	0	18560	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (444) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:3236:HTL:C2	5:B:3236:HTL:C1'	1.94	1.43
5:A:2236:HTL:C2	5:A:2236:HTL:C1'	1.97	1.39
1:A:635:THR:HG22	1:A:640:LYS:HE2	1.34	1.05
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.23	0.98
1:A:1129:MET:HE3	1:A:1149:ARG:HD3	1.48	0.95
1:B:883:MET:HE3	1:B:887:ARG:HD2	1.51	0.91
1:A:841:SER:HB3	1:A:989:MET:HE1	1.53	0.90
1:A:892:ASP:HB3	7:A:2415:HOH:O	1.70	0.90
1:A:1132:ASN:HD21	1:A:1139:ARG:HH12	1.21	0.89
1:B:554:GLY:HA3	1:B:601:MET:HE2	1.55	0.89
1:A:398:VAL:HG13	1:A:656:VAL:HG22	1.54	0.88
1:A:1181:LYS:H	1:B:1019:ARG:HH12	1.22	0.87
1:A:883:MET:SD	7:B:3601:HOH:O	2.34	0.86
1:B:874:GLU:HB3	7:B:4242:HOH:O	1.75	0.86
1:A:1219:THR:HG21	7:B:3370:HOH:O	1.77	0.83
1:B:1200:THR:HG23	1:B:1202:MET:H	1.42	0.83
1:A:147:GLN:HE22	1:A:184:GLU:H	1.25	0.82
1:A:883:MET:HE3	1:A:887:ARG:HD2	1.61	0.81
1:B:227:GLN:H	1:B:227:GLN:HE21	1.28	0.81
1:A:227:GLN:H	1:A:227:GLN:HE21	1.29	0.80
1:A:532:ARG:CA	1:A:533:THR:N	2.44	0.80
1:A:601:MET:CA	1:A:602:ASN:N	2.44	0.80
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.28	0.80
1:B:712:GLU:CA	1:B:713:GLU:N	2.45	0.80
1:B:856:ASN:HD21	1:B:860:GLN:HE21	1.27	0.80
1:B:1129:MET:HE3	1:B:1149:ARG:HD3	1.62	0.79
1:B:6:MET:HE2	1:B:185:VAL:HG11	1.65	0.79
1:B:147:GLN:HE22	1:B:184:GLU:H	1.32	0.78
1:B:1189:GLY:HA3	1:B:1196:THR:HG21	1.66	0.77
1:A:396:ASP:HA	1:A:656:VAL:HG13	1.65	0.77
1:A:1200:THR:HG23	1:A:1202:MET:HE3	1.66	0.76
1:B:883:MET:HE2	1:B:955:LYS:HG3	1.68	0.75
1:B:1173:GLU:HA	7:B:3899:HOH:O	1.86	0.75
1:B:396:ASP:HA	1:B:656:VAL:HG13	1.67	0.75
7:A:2814:HOH:O	1:B:883:MET:SD	2.45	0.75
1:A:535:ALA:HB1	1:A:623:LYS:HG3	1.70	0.74
1:A:765:GLN:HE22	1:B:1229:ARG:HH12	1.36	0.73
1:B:712:GLU:CA	1:B:712:GLU:O	2.35	0.73
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.37	0.72
1:A:1107:ALA:HB2	1:A:1175:PHE:HB3	1.71	0.72
1:A:1080:MET:H	1:B:1215:ASN:ND2	1.88	0.72
1:B:608:GLN:HG3	7:B:4160:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HG2	7:B:4207:HOH:O	1.90	0.71
1:A:601:MET:CA	1:A:601:MET:O	2.39	0.71
1:A:198:LYS:H	1:A:198:LYS:HZ3	1.36	0.70
1:A:643:VAL:HB	1:A:849:PRO:HB2	1.71	0.70
1:A:856:ASN:HD21	1:A:860:GLN:HE21	1.39	0.70
1:A:325:THR:HG21	7:A:2328:HOH:O	1.92	0.70
1:B:1189:GLY:CA	1:B:1196:THR:HG21	2.22	0.70
1:A:532:ARG:CA	1:A:532:ARG:O	2.40	0.70
1:B:549:ILE:HG23	1:B:608:GLN:HG2	1.73	0.69
1:B:1129:MET:HA	1:B:1129:MET:HE2	1.75	0.69
1:B:198:LYS:H	1:B:198:LYS:HD2	1.57	0.69
1:A:1200:THR:HG21	7:A:2647:HOH:O	1.92	0.69
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.73	0.69
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.41	0.69
1:B:1198:ASP:OD2	1:B:1200:THR:HB	1.92	0.69
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.57	0.68
7:A:2929:HOH:O	1:B:1180:GLY:HA3	1.94	0.68
1:B:5:MET:HE1	1:B:184:GLU:HB2	1.75	0.68
1:A:1215:ASN:ND2	1:B:1080:MET:H	1.91	0.68
1:B:986:VAL:HG22	1:B:1064:LEU:HD23	1.75	0.67
1:A:1219:THR:HG22	1:A:1222:GLN:N	2.05	0.67
1:A:765:GLN:NE2	1:B:1229:ARG:HH12	1.92	0.67
1:B:636:ASN:HB3	1:B:639:PHE:H	1.60	0.67
1:A:463:ILE:HD11	1:A:465:ILE:HG22	1.76	0.67
1:A:883:MET:CE	1:A:887:ARG:HD2	2.25	0.67
1:A:1200:THR:HG23	1:A:1202:MET:H	1.60	0.67
1:A:1198:ASP:OD2	1:A:1200:THR:HB	1.94	0.67
1:A:1077:ARG:HH11	1:A:1077:ARG:HB2	1.58	0.66
1:B:509:THR:HG21	7:B:3646:HOH:O	1.95	0.66
1:A:509:THR:HG21	7:A:2978:HOH:O	1.96	0.66
1:A:55:THR:HG22	7:A:2794:HOH:O	1.94	0.66
1:A:1028:MET:HE2	1:B:1028:MET:HE2	1.78	0.66
1:B:325:THR:HG21	7:B:3257:HOH:O	1.95	0.66
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.97	0.65
1:A:416:GLY:C	7:A:3044:HOH:O	2.39	0.65
1:A:606:VAL:O	1:A:610:VAL:HG23	1.97	0.65
1:A:986:VAL:HG22	1:A:1064:LEU:HD23	1.78	0.65
1:B:891:ALA:HB2	1:B:917:LYS:HZ1	1.62	0.64
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.77	0.64
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.96	0.64
1:A:444:ASN:HB2	1:A:582:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:HB	1:B:180:ILE:HD11	1.79	0.62
1:B:10:GLY:O	1:B:14:THR:HG23	2.00	0.62
1:A:8:THR:HG22	7:A:2981:HOH:O	1.99	0.62
1:A:24:VAL:HG13	1:B:881:MET:HE2	1.80	0.62
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.35	0.62
1:A:642:VAL:C	1:A:645:PRO:HD2	2.25	0.62
1:A:881:MET:HE2	1:B:24:VAL:HG13	1.80	0.62
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.65	0.61
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.80	0.61
1:A:1162:GLU:HG2	7:B:4112:HOH:O	1.98	0.61
1:A:1189:GLY:CA	1:A:1196:THR:HG21	2.29	0.61
1:A:635:THR:HG23	1:A:639:PHE:HB3	1.83	0.61
1:B:780:TYR:HA	1:B:783:ARG:HH11	1.66	0.60
1:A:841:SER:CB	1:A:989:MET:HE1	2.30	0.59
1:A:1129:MET:HE3	1:A:1149:ARG:CD	2.28	0.59
1:A:1080:MET:H	1:B:1215:ASN:HD21	1.51	0.59
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.83	0.59
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.17	0.59
1:B:821:VAL:HG13	1:B:989:MET:HE1	1.83	0.59
1:B:9:ASP:OD2	1:B:12:THR:HG23	2.01	0.59
1:B:311:GLU:HB3	7:B:4077:HOH:O	2.00	0.59
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.84	0.59
1:B:398:VAL:HG13	1:B:656:VAL:HG22	1.84	0.59
1:B:5:MET:CE	1:B:184:GLU:HB2	2.32	0.59
1:A:691:GLN:HE22	1:A:727:LYS:H	1.51	0.59
1:B:821:VAL:CG1	1:B:989:MET:HE1	2.33	0.59
1:B:110:HIS:HE1	1:B:157:HIS:NE2	2.01	0.58
1:A:1054:LYS:HB2	7:A:2568:HOH:O	2.02	0.58
1:A:351:ARG:HD2	7:A:2281:HOH:O	2.03	0.58
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.02	0.58
1:B:1187:ASP:HB3	1:B:1190:GLU:HG3	1.85	0.57
1:A:1200:THR:CG2	1:A:1202:MET:HE3	2.34	0.57
1:B:1200:THR:CG2	1:B:1202:MET:HE3	2.34	0.57
7:A:2421:HOH:O	1:B:953:THR:HG21	2.04	0.57
1:B:883:MET:CE	1:B:887:ARG:HD2	2.29	0.57
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	2.04	0.57
1:A:273:ILE:HG23	1:A:327:LEU:HD22	1.87	0.57
1:A:325:THR:HG23	1:A:382:MET:SD	2.45	0.57
1:A:16:HIS:HD2	7:A:2251:HOH:O	1.87	0.57
1:B:43:TRP:HB3	1:B:48:ARG:HD2	1.87	0.57
1:B:779:GLU:C	1:B:783:ARG:HH11	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:GLN:NE2	1:A:727:LYS:H	2.02	0.56
1:B:601:MET:HE1	7:B:3967:HOH:O	2.05	0.56
1:A:644:LYS:N	1:A:645:PRO:CD	2.68	0.56
1:B:698:VAL:HG22	1:B:1084:GLN:CD	2.30	0.56
1:A:883:MET:HE2	1:A:955:LYS:CG	2.35	0.56
1:B:737:ARG:HE	1:B:739:GLN:NE2	2.02	0.56
1:A:953:THR:HG21	7:B:3491:HOH:O	2.06	0.56
1:A:1189:GLY:HA3	1:A:1196:THR:HG21	1.87	0.56
1:B:883:MET:HE2	1:B:955:LYS:CG	2.34	0.56
1:B:467:HIS:CD2	1:B:481:VAL:H	2.24	0.56
1:A:398:VAL:CG1	1:A:656:VAL:HG22	2.32	0.56
1:A:227:GLN:H	1:A:227:GLN:NE2	2.00	0.55
1:A:686:PRO:HB2	1:A:724:LEU:HD21	1.87	0.55
1:A:1123:SER:O	1:A:1126:GLU:HG2	2.06	0.55
1:B:780:TYR:HA	1:B:783:ARG:HD2	1.87	0.55
1:B:871:ASP:O	1:B:874:GLU:HG2	2.06	0.55
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.87	0.55
1:B:16:HIS:HD2	7:B:3275:HOH:O	1.87	0.55
1:B:456:ASP:OD1	1:B:463:ILE:HG22	2.06	0.55
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.88	0.55
1:A:10:GLY:O	1:A:14:THR:HG23	2.06	0.55
1:A:467:HIS:CD2	1:A:481:VAL:H	2.25	0.55
1:A:630:LYS:C	1:A:632:GLU:H	2.14	0.55
1:A:1028:MET:HE3	1:B:1028:MET:HB3	1.88	0.55
1:A:418:ILE:HD12	1:A:418:ILE:N	2.22	0.54
1:A:950:ASP:OD2	1:B:212:HIS:HE1	1.89	0.54
1:A:1166:MET:O	1:A:1169:THR:HG22	2.06	0.54
1:B:14:THR:HG21	1:B:171:PHE:CE2	2.43	0.54
1:B:91:LEU:HD11	1:B:116:ILE:HD12	1.90	0.54
1:B:1132:ASN:O	1:B:1136:VAL:HG22	2.08	0.54
1:B:14:THR:HG22	1:B:149:ALA:HB1	1.89	0.54
1:A:1181:LYS:H	1:B:1019:ARG:NH1	1.99	0.54
1:A:9:ASP:OD2	1:A:12:THR:HG23	2.07	0.54
1:A:775:VAL:N	1:A:776:PRO:HD2	2.23	0.54
1:A:411:ASP:HB2	1:A:483:ARG:HD2	1.89	0.54
1:A:821:VAL:HG21	1:A:844:TRP:CH2	2.43	0.53
1:A:635:THR:HG23	1:A:636:ASN:H	1.73	0.53
1:A:135:GLN:H	1:A:135:GLN:NE2	2.06	0.53
1:A:7:THR:HB	1:A:180:ILE:HD11	1.90	0.53
1:B:212:HIS:HD2	7:B:3461:HOH:O	1.91	0.53
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ARG:HE	1:A:739:GLN:NE2	2.06	0.53
1:A:927:GLY:O	1:A:931:LYS:HG3	2.08	0.53
1:B:805:LEU:HB2	1:B:825:THR:HB	1.91	0.53
1:A:817:GLU:CD	1:A:989:MET:HE3	2.34	0.53
1:A:1003:LYS:HZ3	1:B:976:HIS:HD2	1.57	0.53
1:A:697:PHE:CD2	1:A:1046:LYS:HD3	2.44	0.52
1:A:1111:ASN:HD21	1:A:1169:THR:HG23	1.74	0.52
1:B:544:ILE:HD12	1:B:613:LEU:HD13	1.91	0.52
1:B:775:VAL:HB	1:B:776:PRO:HD3	1.91	0.52
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.91	0.52
1:A:444:ASN:CB	1:A:582:LEU:HD21	2.39	0.52
1:B:325:THR:HG23	1:B:382:MET:HE2	1.91	0.52
1:B:509:THR:HG22	7:B:3921:HOH:O	2.09	0.52
1:B:780:TYR:CA	1:B:783:ARG:HH11	2.22	0.52
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.90	0.52
1:B:1200:THR:CG2	1:B:1202:MET:H	2.20	0.52
1:B:1035:VAL:HG22	1:B:1062:PRO:HG2	1.92	0.52
1:B:691:GLN:NE2	1:B:727:LYS:H	2.07	0.52
1:B:1200:THR:HG23	1:B:1202:MET:HE3	1.91	0.52
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.91	0.51
1:B:351:ARG:HD2	7:B:3509:HOH:O	2.10	0.51
1:A:456:ASP:HB2	7:B:3660:HOH:O	2.10	0.51
1:A:1189:GLY:HA2	1:A:1196:THR:HG21	1.90	0.51
1:B:1129:MET:HE3	1:B:1149:ARG:CD	2.34	0.51
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.92	0.51
1:A:350:GLU:CD	1:B:389:HIS:HE1	2.19	0.51
1:B:135:GLN:H	1:B:135:GLN:NE2	2.09	0.51
1:B:390:PHE:CD1	1:B:403:LEU:HD22	2.46	0.51
1:B:1198:ASP:OD1	1:B:1203:MET:HE3	2.11	0.51
1:A:212:HIS:HD2	7:A:2694:HOH:O	1.94	0.51
1:B:989:MET:SD	7:B:3942:HOH:O	2.59	0.51
1:B:1077:ARG:HH11	1:B:1077:ARG:HB2	1.76	0.51
1:B:691:GLN:HE22	1:B:727:LYS:H	1.59	0.51
1:B:536:ASN:HD22	1:B:623:LYS:NZ	2.09	0.51
1:A:636:ASN:HB3	1:A:638:PHE:H	1.76	0.50
1:A:1111:ASN:ND2	1:A:1169:THR:HG23	2.26	0.50
1:B:948:MET:HE2	1:B:951:LEU:HD12	1.94	0.50
1:A:953:THR:HG22	7:A:2274:HOH:O	2.11	0.50
1:B:1029:VAL:HG22	1:B:1037:VAL:CG2	2.41	0.50
1:A:5:MET:HE1	1:A:184:GLU:HB2	1.94	0.50
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:MET:HE1	1:A:583:LEU:HD22	1.94	0.50
1:A:918:ASN:O	1:A:954:LYS:HD2	2.12	0.50
1:A:7:THR:OG1	1:A:439:LYS:HE3	2.11	0.50
1:B:637:GLU:HG2	1:B:638:PHE:N	2.27	0.50
1:B:233:ASN:HB2	1:B:234:PRO:HD3	1.92	0.49
1:B:1029:VAL:HG22	1:B:1037:VAL:HG22	1.93	0.49
1:A:561:MET:HE1	1:A:583:LEU:CD2	2.43	0.49
1:B:322:LYS:O	1:B:356:PRO:O	2.29	0.49
1:B:636:ASN:HB2	1:B:639:PHE:HB2	1.93	0.49
1:A:756:PRO:N	1:A:757:PRO:HD2	2.27	0.49
1:B:1000:GLN:HG3	1:B:1012:LYS:HB2	1.94	0.49
7:A:2819:HOH:O	1:B:1221:GLU:HG2	2.12	0.49
1:A:467:HIS:HD2	1:A:481:VAL:H	1.59	0.49
1:A:16:HIS:HE1	1:A:186:LEU:O	1.96	0.49
1:A:227:GLN:HE21	1:A:227:GLN:N	2.05	0.49
1:A:110:HIS:CD2	1:A:169:HIS:HD2	2.26	0.49
1:A:463:ILE:CD1	1:A:465:ILE:HG22	2.43	0.49
1:B:718:PRO:HG2	1:B:777:ASN:HD22	1.77	0.49
1:A:135:GLN:HG2	7:A:2668:HOH:O	2.12	0.49
1:A:773:ALA:O	1:A:776:PRO:HD2	2.13	0.48
1:A:1202:MET:HG2	6:B:3240:CO2:O2	2.13	0.48
1:B:431:VAL:CG2	1:B:464:THR:HG21	2.43	0.48
1:A:59:ARG:HG2	1:B:881:MET:HE3	1.93	0.48
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.43	0.48
1:A:389:HIS:HE1	1:B:350:GLU:CD	2.21	0.48
1:A:818:THR:HA	1:A:821:VAL:HG22	1.95	0.48
1:A:1111:ASN:HD21	1:A:1169:THR:CG2	2.26	0.48
1:B:467:HIS:HD2	1:B:481:VAL:H	1.59	0.48
1:B:1146:LYS:HD3	7:B:3988:HOH:O	2.12	0.48
1:A:389:HIS:HD2	7:A:2627:HOH:O	1.97	0.48
1:A:780:TYR:HA	1:A:783:ARG:HD2	1.95	0.48
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.48	0.48
1:A:351:ARG:NH1	1:A:354:ALA:O	2.47	0.48
1:B:639:PHE:CE1	1:B:643:VAL:HG22	2.48	0.48
1:A:1154:HIS:HE1	1:B:1174:SER:HB2	1.78	0.48
1:A:1199:ASP:CG	1:A:1214:GLN:HE22	2.21	0.48
1:A:8:THR:HG21	1:A:12:THR:OG1	2.14	0.48
1:A:569:LYS:NZ	1:A:610:VAL:O	2.47	0.48
1:A:473:LYS:HB3	1:A:474:PRO:HD2	1.96	0.48
1:A:1219:THR:CG2	1:A:1221:GLU:HG2	2.44	0.48
1:B:3:LYS:HB3	1:B:184:GLU:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:HIS:CD2	1:B:169:HIS:HD2	2.26	0.47
1:B:953:THR:HG22	7:B:3279:HOH:O	2.14	0.47
1:A:909:ALA:CB	1:A:930:LEU:HD13	2.44	0.47
1:B:594:LYS:N	7:B:3668:HOH:O	2.47	0.47
1:A:331:LYS:HD3	1:A:362:ARG:CZ	2.45	0.47
1:A:1185:SER:HB3	1:B:45:ALA:HB3	1.95	0.47
7:A:2345:HOH:O	1:B:229:ARG:HD2	2.15	0.47
1:A:27:ILE:HG13	7:A:2418:HOH:O	2.13	0.47
1:A:821:VAL:HG21	1:A:844:TRP:HH2	1.79	0.47
1:B:198:LYS:HD2	1:B:198:LYS:N	2.28	0.47
1:A:805:LEU:HB2	1:A:825:THR:HB	1.96	0.47
1:A:507:GLY:HA2	1:A:538:LYS:O	2.15	0.47
1:B:1040:VAL:HG12	1:B:1048:GLN:HE22	1.80	0.47
1:B:779:GLU:C	1:B:783:ARG:NH1	2.72	0.47
1:B:874:GLU:CD	7:B:4242:HOH:O	2.58	0.47
1:A:273:ILE:CG2	1:A:327:LEU:HD22	2.45	0.47
1:A:90:LEU:HD11	1:A:168:MET:CE	2.46	0.46
1:A:390:PHE:CD1	1:A:403:LEU:HD22	2.49	0.46
1:B:910:LEU:HD13	1:B:930:LEU:HD11	1.96	0.46
1:A:390:PHE:CE1	1:A:403:LEU:HD22	2.51	0.46
1:A:650:GLN:CD	1:A:653:LYS:HE3	2.39	0.46
1:A:1186:VAL:HG23	1:A:1190:GLU:OE1	2.15	0.46
1:B:1042:MET:HG2	1:B:1084:GLN:HE22	1.80	0.46
1:A:240:PRO:HB3	1:A:309:VAL:HG21	1.97	0.46
1:A:12:THR:HB	1:A:39:GLU:OE2	2.15	0.46
1:A:9:ASP:HA	1:A:179:GLU:O	2.15	0.46
1:A:342:LEU:HD12	1:B:346:SER:HB3	1.97	0.46
1:A:465:ILE:HG13	1:A:467:HIS:CE1	2.51	0.46
1:A:739:GLN:NE2	1:A:777:ASN:HB3	2.31	0.46
1:B:802:GLN:NE2	7:B:4051:HOH:O	2.43	0.46
1:A:775:VAL:N	1:A:776:PRO:CD	2.79	0.46
1:A:841:SER:HA	1:A:844:TRP:CE2	2.51	0.46
1:B:544:ILE:CD1	1:B:613:LEU:HD13	2.46	0.46
1:A:90:LEU:HD21	1:A:168:MET:HE1	1.97	0.46
1:B:732:LYS:CD	1:B:732:LYS:CA	2.93	0.46
1:B:883:MET:CE	1:B:955:LYS:HG3	2.42	0.46
1:B:1197:ARG:HD3	7:B:4066:HOH:O	2.16	0.46
1:A:108:VAL:HG21	1:A:157:HIS:HA	1.98	0.45
1:A:325:THR:CG2	1:A:382:MET:SD	3.04	0.45
1:A:421:GLN:NE2	7:A:2725:HOH:O	2.50	0.45
1:A:729:LYS:O	1:A:732:LYS:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	2.13	0.45
1:A:1077:ARG:HD2	7:A:3041:HOH:O	2.16	0.45
1:A:355:MET:HA	1:A:356:PRO:HD2	1.86	0.45
1:A:588:HIS:CD2	1:A:599:VAL:HG11	2.51	0.45
1:A:90:LEU:HD11	1:A:168:MET:HE1	1.98	0.45
1:A:639:PHE:CE1	1:A:672:PHE:HB2	2.51	0.45
1:B:227:GLN:H	1:B:227:GLN:NE2	2.05	0.45
1:A:764:MET:C	1:A:765:GLN:HG2	2.41	0.45
1:A:775:VAL:O	1:A:779:GLU:HG2	2.16	0.45
1:B:841:SER:HA	1:B:844:TRP:CE2	2.51	0.45
1:A:989:MET:HE2	1:A:989:MET:HB2	1.92	0.45
1:A:730:GLU:CD	1:A:730:GLU:H	2.24	0.45
1:B:1104:ARG:HB2	7:B:4216:HOH:O	2.16	0.45
1:A:1231:LYS:O	1:A:1232:LYS:HB2	2.17	0.45
1:B:423:TRP:CE3	1:B:463:ILE:HD11	2.52	0.45
1:B:780:TYR:N	1:B:783:ARG:HH11	2.14	0.45
1:A:818:THR:OG1	1:A:819:PRO:HD3	2.17	0.45
1:B:1104:ARG:O	1:B:1108:GLN:HG3	2.17	0.45
1:B:465:ILE:HG13	1:B:467:HIS:CE1	2.52	0.45
1:A:221:ASN:HB3	1:A:222:PRO:HD2	2.00	0.44
1:B:389:HIS:HD2	7:B:3639:HOH:O	2.00	0.44
1:A:198:LYS:HZ3	1:A:198:LYS:N	2.10	0.44
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.47	0.44
1:A:497:ILE:HG13	1:A:498:TYR:CD1	2.53	0.44
1:A:1078:LYS:O	1:B:1219:THR:HG23	2.18	0.44
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.83	0.44
1:A:560:ASN:H	1:A:560:ASN:HD22	1.65	0.44
1:B:1199:ASP:CG	1:B:1214:GLN:HE22	2.26	0.44
1:A:883:MET:HE2	1:A:955:LYS:HG3	2.00	0.44
1:B:578:LYS:HG2	1:B:582:LEU:HD22	1.98	0.44
1:A:268:ASP:OD2	1:A:296:LYS:NZ	2.38	0.44
1:A:357:LYS:HE3	1:A:359:LEU:HD13	1.98	0.44
1:A:1196:THR:HG22	7:A:2483:HOH:O	2.16	0.44
1:A:1198:ASP:OD1	1:A:1203:MET:HE3	2.18	0.44
1:B:1177:PRO:O	1:B:1178:ALA:HB2	2.17	0.44
1:B:495:VAL:HG13	1:B:527:PRO:HD3	2.00	0.44
1:A:1143:GLU:HG2	7:A:3066:HOH:O	2.18	0.44
1:A:1219:THR:CG2	1:A:1222:GLN:H	2.11	0.44
1:A:465:ILE:HG12	7:A:2473:HOH:O	2.17	0.44
1:A:554:GLY:C	1:A:556:GLY:H	2.26	0.43
1:A:576:PHE:O	1:A:580:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:ASN:HA	1:B:623:LYS:HZ3	1.83	0.43
1:A:635:THR:HG23	1:A:636:ASN:N	2.33	0.43
1:B:871:ASP:HB2	1:B:874:GLU:HG2	1.99	0.43
1:A:82:THR:HG22	1:A:108:VAL:O	2.18	0.43
1:A:650:GLN:OE1	1:A:653:LYS:HE3	2.19	0.43
1:B:27:ILE:HD11	1:B:84:PHE:CD1	2.54	0.43
1:B:739:GLN:NE2	1:B:777:ASN:HB3	2.34	0.43
1:A:487:VAL:O	1:A:510:PHE:HA	2.19	0.43
1:B:906:VAL:HG12	1:B:910:LEU:HD22	2.00	0.43
1:A:1219:THR:HG23	1:A:1221:GLU:HG2	2.00	0.43
1:B:491:ASN:HD22	1:B:492:PRO:HD2	1.82	0.43
1:B:644:LYS:N	1:B:645:PRO:CD	2.82	0.43
1:B:821:VAL:CG1	1:B:989:MET:CE	2.96	0.43
1:A:180:ILE:HD12	1:A:181:GLN:N	2.34	0.43
1:A:806:MET:HE2	1:A:821:VAL:CG2	2.48	0.43
1:B:775:VAL:N	1:B:776:PRO:CD	2.82	0.43
1:A:574:LEU:HD13	1:A:578:LYS:HG2	2.01	0.43
1:A:590:ALA:O	1:A:591:TYR:HB2	2.18	0.43
1:A:639:PHE:CE1	1:A:643:VAL:HG22	2.53	0.43
1:A:1215:ASN:HD21	1:B:1079:GLY:HA2	1.84	0.43
1:B:630:LYS:C	1:B:632:GLU:H	2.27	0.43
1:B:1200:THR:HG22	1:B:1203:MET:H	1.83	0.43
1:A:357:LYS:HD2	7:A:2763:HOH:O	2.18	0.42
1:A:534:ILE:HA	1:A:539:LEU:HD12	2.01	0.42
1:A:601:MET:N	1:A:602:ASN:N	2.67	0.42
1:B:779:GLU:O	1:B:783:ARG:HD2	2.19	0.42
1:B:1219:THR:O	1:B:1223:GLN:HG3	2.19	0.42
1:A:331:LYS:HD2	7:A:2573:HOH:O	2.19	0.42
1:A:1111:ASN:CG	7:A:3084:HOH:O	2.62	0.42
1:A:1200:THR:CG2	1:A:1202:MET:HB2	2.50	0.42
1:A:1229:ARG:HH12	1:B:765:GLN:HE22	1.67	0.42
1:A:1030:MET:HE1	1:A:1099:PHE:CE1	2.54	0.42
1:B:891:ALA:CB	1:B:917:LYS:HZ1	2.28	0.42
1:B:1165:HIS:O	1:B:1165:HIS:CG	2.72	0.42
1:A:61:MET:HG3	1:A:67:ALA:HA	2.01	0.42
1:A:561:MET:HE2	1:A:587:ILE:HD11	2.00	0.42
1:B:141:LEU:HD13	1:B:152:MET:HB3	2.01	0.42
1:A:1028:MET:CE	1:B:1028:MET:HB3	2.49	0.42
1:B:37:GLY:HA3	7:B:4020:HOH:O	2.20	0.42
1:A:61:MET:HA	1:B:976:HIS:CE1	2.54	0.42
1:B:574:LEU:HB3	1:B:575:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:THR:CG2	1:A:39:GLU:OE2	2.68	0.42
1:A:562:ILE:HD12	1:A:562:ILE:N	2.35	0.42
1:A:681:VAL:HB	1:A:682:PRO:HD2	2.00	0.42
1:A:806:MET:HE2	1:A:821:VAL:HG23	2.01	0.42
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.50	0.42
1:B:699:CYS:HA	1:B:700:PRO:HD3	1.80	0.42
1:A:617:LYS:HD3	1:A:617:LYS:HA	1.80	0.42
1:A:754:ILE:HD13	1:A:1084:GLN:HB2	2.02	0.42
1:B:536:ASN:HD22	1:B:623:LYS:HZ3	1.66	0.42
1:B:779:GLU:HB3	1:B:783:ARG:NH1	2.35	0.42
1:B:1166:MET:O	1:B:1169:THR:HG22	2.20	0.42
1:A:2:GLY:N	1:A:187:ASP:OD2	2.53	0.42
1:B:61:MET:HG3	1:B:67:ALA:HA	2.01	0.42
1:B:566:ALA:O	1:B:570:LEU:HB2	2.19	0.42
1:B:140:MET:HG2	1:B:168:MET:HE3	2.01	0.41
1:A:584:LYS:HA	1:A:587:ILE:HD12	2.02	0.41
1:B:238:LYS:HZ2	1:B:238:LYS:HG3	1.63	0.41
1:A:152:MET:HE3	1:A:303:ARG:HG3	2.02	0.41
1:B:87:SER:HA	1:B:129:ASP:HB3	2.01	0.41
1:A:717:ALA:HA	1:A:718:PRO:HD3	1.91	0.41
1:B:750:ASN:HD21	1:B:1083:SER:HB2	1.86	0.41
1:B:779:GLU:HB3	1:B:783:ARG:HH12	1.86	0.41
1:A:233:ASN:HD21	1:B:331:LYS:HE3	1.84	0.41
1:A:289:HIS:HE1	7:A:3078:HOH:O	2.03	0.41
1:A:507:GLY:N	1:A:537:LYS:O	2.51	0.41
1:A:976:HIS:CE1	1:B:61:MET:HA	2.56	0.41
1:A:1229:ARG:HH12	1:B:765:GLN:NE2	2.18	0.41
1:B:1026:ALA:O	1:B:1030:MET:HG3	2.20	0.41
1:A:289:HIS:HD2	7:A:2635:HOH:O	2.03	0.41
1:A:1174:SER:HB2	1:B:1154:HIS:HE1	1.86	0.41
1:A:1180:GLY:H	1:A:1181:LYS:HZ1	1.67	0.41
1:B:12:THR:CG2	1:B:39:GLU:OE2	2.69	0.41
1:B:569:LYS:HG2	1:B:570:LEU:HD13	2.02	0.41
1:B:737:ARG:HH11	1:B:739:GLN:HE22	1.68	0.41
1:B:934:LEU:HD22	1:B:942:LEU:HG	2.03	0.41
1:A:909:ALA:HB1	1:A:930:LEU:HD13	2.01	0.41
1:A:1118:LYS:HE3	7:A:2370:HOH:O	2.21	0.41
1:B:754:ILE:HD13	1:B:1084:GLN:HB2	2.02	0.41
1:A:5:MET:HE1	7:A:3054:HOH:O	2.20	0.41
1:A:20:ALA:HB2	1:A:188:TYR:CE1	2.56	0.41
1:A:35:THR:O	1:A:39:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HE3	7:A:2963:HOH:O	2.21	0.41
5:A:2236:HTL:C1'	6:A:2240:CO2:C	2.99	0.41
5:A:2236:HTL:H5A1	5:A:2236:HTL:H4A1	1.56	0.41
1:B:7:THR:OG1	1:B:439:LYS:HE3	2.21	0.41
1:B:184:GLU:HG2	1:B:185:VAL:N	2.36	0.41
1:B:268:ASP:OD2	1:B:296:LYS:NZ	2.44	0.41
1:B:667:LEU:HB3	1:B:854:LYS:HA	2.01	0.41
1:B:1176:ALA:HA	1:B:1177:PRO:HD3	1.90	0.41
5:B:3236:HTL:H4A3	5:B:3236:HTL:H351	1.90	0.41
1:B:108:VAL:HG21	1:B:157:HIS:HA	2.02	0.41
1:B:426:GLY:O	1:B:427:ALA:HB3	2.21	0.41
1:B:576:PHE:HA	7:B:4071:HOH:O	2.21	0.41
1:B:635:THR:HG21	7:B:4182:HOH:O	2.21	0.41
1:B:637:GLU:CG	1:B:638:PHE:N	2.84	0.41
1:B:765:GLN:HA	1:B:765:GLN:HE21	1.86	0.41
1:A:784:ILE:HA	1:A:785:PRO:HD3	1.90	0.40
1:A:822:ARG:HD3	7:A:2300:HOH:O	2.21	0.40
1:A:883:MET:HE2	1:A:955:LYS:HG2	2.04	0.40
1:A:491:ASN:HA	1:A:492:PRO:HD2	1.83	0.40
7:A:2543:HOH:O	1:B:1200:THR:HG21	2.20	0.40
1:B:755:CYS:O	1:B:760:LYS:NZ	2.52	0.40
1:A:229:ARG:HD2	7:B:3789:HOH:O	2.20	0.40
1:A:250:VAL:HG12	7:A:2605:HOH:O	2.22	0.40
1:A:667:LEU:HB3	1:A:854:LYS:HA	2.02	0.40
1:B:781:ALA:HA	1:B:784:ILE:HD12	2.02	0.40
1:A:671:GLN:NE2	1:A:854:LYS:HD2	2.36	0.40
1:B:16:HIS:HE1	1:B:186:LEU:O	2.05	0.40
1:B:840:CYS:SG	1:B:996:ASN:HB2	2.62	0.40
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.57	0.40
1:A:283:ILE:HG21	1:A:299:LEU:HD13	2.04	0.40
1:A:705:LEU:HA	1:A:706:PRO:HD3	1.95	0.40
1:A:1202:MET:HE3	1:A:1202:MET:HB2	1.94	0.40
1:B:1076:LEU:HB3	7:B:4233:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1229/1231 (100%)	1181 (96%)	42 (3%)	6 (0%)	24	16
1	B	1229/1231 (100%)	1191 (97%)	33 (3%)	5 (0%)	30	22
All	All	2458/2462 (100%)	2372 (96%)	75 (3%)	11 (0%)	30	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	LYS
1	B	732	LYS
1	B	1178	ALA
1	A	732	LYS
1	A	1178	ALA
1	A	1181	LYS
1	B	1181	LYS
1	B	1231	LYS
1	A	1231	LYS
1	A	631	ALA
1	B	357	LYS

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%)	850 (87%)	128 (13%)	4	1
1	B	978/978 (100%)	855 (87%)	123 (13%)	4	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1956/1956 (100%)	1705 (87%)	251 (13%)	4 1

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	8	THR
1	A	12	THR
1	A	14	THR
1	A	27	ILE
1	A	82	THR
1	A	111	VAL
1	A	141	LEU
1	A	154	LEU
1	A	180	ILE
1	A	181	GLN
1	A	184	GLU
1	A	194	LEU
1	A	198	LYS
1	A	204	ARG
1	A	215	VAL
1	A	227	GLN
1	A	239	VAL
1	A	245	GLU
1	A	260	LEU
1	A	264	VAL
1	A	290	LEU
1	A	302	VAL
1	A	317	LEU
1	A	324	ILE
1	A	325	THR
1	A	327	LEU
1	A	342	LEU
1	A	349	VAL
1	A	351	ARG
1	A	355	MET
1	A	359	LEU
1	A	377	SER
1	A	392	VAL
1	A	398	VAL
1	A	403	LEU
1	A	415	LYS

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Mol	Chain	Res	Type
1	A	439	LYS
1	A	456	ASP
1	A	463	ILE
1	A	465	ILE
1	A	495	VAL
1	A	501	LEU
1	A	509	THR
1	A	511	VAL
1	A	513	ASN
1	A	518	SER
1	A	532	ARG
1	A	548	LYS
1	A	558	ARG
1	A	560	ASN
1	A	570	LEU
1	A	573	VAL
1	A	577	GLU
1	A	582	LEU
1	A	583	LEU
1	A	586	SER
1	A	593	LYS
1	A	594	LYS
1	A	612	SER
1	A	613	LEU
1	A	621	SER
1	A	630	LYS
1	A	632	GLU
1	A	635	THR
1	A	637	GLU
1	A	640	LYS
1	A	643	VAL
1	A	654	LEU
1	A	656	VAL
1	A	687	GLU
1	A	710	LYS
1	A	714	LEU
1	A	720	ASN
1	A	727	LYS
1	A	729	LYS
1	A	732	LYS
1	A	754	ILE
1	A	758	LYS

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Mol	Chain	Res	Type
1	A	759	GLU
1	A	765	GLN
1	A	768	ASP
1	A	778	LEU
1	A	783	ARG
1	A	789	GLU
1	A	790	VAL
1	A	805	LEU
1	A	813	SER
1	A	823	VAL
1	A	831	ARG
1	A	849	PRO
1	A	858	LEU
1	A	880	ASN
1	A	893	LEU
1	A	910	LEU
1	A	914	LEU
1	A	917	LYS
1	A	930	LEU
1	A	938	LYS
1	A	953	THR
1	A	986	VAL
1	A	989	MET
1	A	993	VAL
1	A	997	THR
1	A	1000	GLN
1	A	1029	VAL
1	A	1047	GLN
1	A	1048	GLN
1	A	1064	LEU
1	A	1077	ARG
1	A	1082	LYS
1	A	1104	ARG
1	A	1124	VAL
1	A	1136	VAL
1	A	1137	LEU
1	A	1140	SER
1	A	1146	LYS
1	A	1170	ASN
1	A	1173	GLU
1	A	1181	LYS
1	A	1183	ASP

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Mol	Chain	Res	Type
1	A	1196	THR
1	A	1200	THR
1	A	1219	THR
1	A	1225	ASP
1	A	1228	LYS
1	A	1231	LYS
1	A	1232	LYS
1	B	11	ASN
1	B	12	THR
1	B	14	THR
1	B	27	ILE
1	B	82	THR
1	B	111	VAL
1	B	141	LEU
1	B	154	LEU
1	B	180	ILE
1	B	181	GLN
1	B	184	GLU
1	B	194	LEU
1	B	211	GLU
1	B	215	VAL
1	B	227	GLN
1	B	238	LYS
1	B	239	VAL
1	B	245	GLU
1	B	248	GLN
1	B	260	LEU
1	B	264	VAL
1	B	290	LEU
1	B	293	LYS
1	B	302	VAL
1	B	311	GLU
1	B	317	LEU
1	B	324	ILE
1	B	325	THR
1	B	327	LEU
1	B	342	LEU
1	B	349	VAL
1	B	351	ARG
1	B	359	LEU
1	B	365	LEU
1	B	383	SER

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Mol	Chain	Res	Type
1	B	392	VAL
1	B	398	VAL
1	B	403	LEU
1	B	439	LYS
1	B	463	ILE
1	B	465	ILE
1	B	472	GLU
1	B	495	VAL
1	B	501	LEU
1	B	509	THR
1	B	511	VAL
1	B	513	ASN
1	B	532	ARG
1	B	570	LEU
1	B	573	VAL
1	B	574	LEU
1	B	582	LEU
1	B	583	LEU
1	B	585	LYS
1	B	593	LYS
1	B	594	LYS
1	B	597	LYS
1	B	613	LEU
1	B	617	LYS
1	B	620	ASP
1	B	628	GLU
1	B	630	LYS
1	B	637	GLU
1	B	643	VAL
1	B	654	LEU
1	B	656	VAL
1	B	687	GLU
1	B	698	VAL
1	B	710	LYS
1	B	714	LEU
1	B	720	ASN
1	B	725	GLU
1	B	729	LYS
1	B	732	LYS
1	B	741	ASN
1	B	754	ILE
1	B	758	LYS

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Mol	Chain	Res	Type
1	B	768	ASP
1	B	778	LEU
1	B	779	GLU
1	B	783	ARG
1	B	789	GLU
1	B	793	ARG
1	B	805	LEU
1	B	813	SER
1	B	821	VAL
1	B	823	VAL
1	B	831	ARG
1	B	854	LYS
1	B	858	LEU
1	B	874	GLU
1	B	880	ASN
1	B	893	LEU
1	B	908	GLU
1	B	910	LEU
1	B	914	LEU
1	B	917	LYS
1	B	930	LEU
1	B	942	LEU
1	B	953	THR
1	B	986	VAL
1	B	993	VAL
1	B	1000	GLN
1	B	1029	VAL
1	B	1047	GLN
1	B	1048	GLN
1	B	1064	LEU
1	B	1077	ARG
1	B	1104	ARG
1	B	1115	LEU
1	B	1118	LYS
1	B	1124	VAL
1	B	1136	VAL
1	B	1137	LEU
1	B	1140	SER
1	B	1162	GLU
1	B	1170	ASN
1	B	1181	LYS
1	B	1196	THR

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Mol	Chain	Res	Type
1	B	1200	THR
1	B	1225	ASP
1	B	1228	LYS
1	B	1232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	96	ASN
1	A	110	HIS
1	A	135	GLN
1	A	147	GLN
1	A	164	ASN
1	A	169	HIS
1	A	181	GLN
1	A	212	HIS
1	A	220	GLN
1	A	227	GLN
1	A	233	ASN
1	A	288	ASN
1	A	289	HIS
1	A	389	HIS
1	A	421	GLN
1	A	467	HIS
1	A	491	ASN
1	A	536	ASN
1	A	543	ASN
1	A	560	ASN
1	A	588	HIS
1	A	602	ASN
1	A	683	GLN
1	A	688	ASN
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	770	GLN
1	A	774	GLN

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Mol	Chain	Res	Type
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	985	ASN
1	A	1000	GLN
1	A	1048	GLN
1	A	1073	ASN
1	A	1084	GLN
1	A	1088	ASN
1	A	1114	GLN
1	A	1132	ASN
1	A	1154	HIS
1	A	1215	ASN
1	A	1223	GLN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	96	ASN
1	B	110	HIS
1	B	135	GLN
1	B	147	GLN
1	B	169	HIS
1	B	181	GLN
1	B	212	HIS
1	B	220	GLN
1	B	221	ASN
1	B	227	GLN
1	B	233	ASN
1	B	288	ASN
1	B	389	HIS
1	B	421	GLN
1	B	434	ASN
1	B	467	HIS
1	B	476	GLN
1	B	491	ASN
1	B	525	HIS
1	B	536	ASN
1	B	560	ASN
1	B	650	GLN

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Mol	Chain	Res	Type
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	765	GLN
1	B	774	GLN
1	B	777	ASN
1	B	836	ASN
1	B	860	GLN
1	B	880	ASN
1	B	918	ASN
1	B	976	HIS
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1084	GLN
1	B	1108	GLN
1	B	1114	GLN
1	B	1132	ASN
1	B	1154	HIS
1	B	1215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no 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	3235	1	0,12,12	-	-	-		
4	SF4	A	2234	1	0,12,12	-	-	-		
5	HTL	B	3236	2	29,30,30	8.21	16 (55%)	35,45,45	2.61	11 (31%)
4	SF4	B	3234	1	0,12,12	-	-	-		
5	HTL	A	2236	2	29,30,30	8.42	16 (55%)	35,45,45	2.92	13 (37%)
4	SF4	B	3233	1	0,12,12	-	-	-		
4	SF4	A	2233	1	0,12,12	-	-	-		
6	CO2	A	2240	-	2,2,2	0.32	0	1,1,1	0.49	0
4	SF4	A	2235	1	0,12,12	-	-	-		
6	CO2	B	3240	-	2,2,2	0.26	0	1,1,1	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	3235	1	-	-	0/6/5/5
4	SF4	A	2234	1	-	-	0/6/5/5
5	HTL	B	3236	2	-	6/19/21/21	0/2/2/2
4	SF4	B	3234	1	-	-	0/6/5/5
5	HTL	A	2236	2	-	6/19/21/21	0/2/2/2
4	SF4	B	3233	1	-	-	0/6/5/5
4	SF4	A	2233	1	-	-	0/6/5/5
4	SF4	A	2235	1	-	-	0/6/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2236	HTL	C1'-C2	40.15	1.97	1.48
5	B	3236	HTL	C1'-C2	37.77	1.94	1.48
5	B	3236	HTL	C4'-N3'	11.10	1.49	1.35
5	A	2236	HTL	C4'-N3'	9.02	1.47	1.35
5	A	2236	HTL	C2'-N1'	8.59	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3236	HTL	C2'-N1'	8.46	1.47	1.34
5	A	2236	HTL	C5'-C4'	8.43	1.56	1.42
5	B	3236	HTL	C4A-C4	-8.28	1.33	1.49
5	B	3236	HTL	C4-N3	-7.71	1.30	1.40
5	A	2236	HTL	C6'-N1'	6.99	1.48	1.34
5	B	3236	HTL	C6'-N1'	6.82	1.48	1.34
5	A	2236	HTL	C2-N3	6.68	1.51	1.34
5	B	3236	HTL	C2-N3	5.71	1.49	1.34
5	A	2236	HTL	C2'-N3'	4.92	1.42	1.34
5	B	3236	HTL	C5'-C4'	4.83	1.50	1.42
5	B	3236	HTL	C5-C4	4.69	1.45	1.35
5	B	3236	HTL	C5-S1	-4.55	1.64	1.74
5	A	2236	HTL	C4'-N4'	4.46	1.45	1.34
5	A	2236	HTL	C3'-C1'	3.92	1.57	1.50
5	A	2236	HTL	C2A-C2'	-3.75	1.39	1.49
5	B	3236	HTL	C35-N3	3.53	1.51	1.47
5	A	2236	HTL	C4A-C4	-3.40	1.42	1.49
5	A	2236	HTL	C2-S1	-2.74	1.62	1.71
5	B	3236	HTL	C4'-N4'	-2.73	1.27	1.34
5	A	2236	HTL	P2-O22	-2.42	1.45	1.54
5	B	3236	HTL	C3'-C1'	2.40	1.54	1.50
5	B	3236	HTL	C2-S1	2.30	1.79	1.71
5	B	3236	HTL	P1-O11	-2.25	1.57	1.59
5	A	2236	HTL	C35-N3	-2.19	1.45	1.47
5	B	3236	HTL	C6'-C5'	2.10	1.41	1.37
5	A	2236	HTL	P1-O11	-2.04	1.57	1.59
5	A	2236	HTL	P1-O13	-2.03	1.45	1.55

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2236	HTL	C5A-C5-S1	-7.63	102.92	119.29
5	A	2236	HTL	C4A-C4-N3	7.41	131.63	121.95
5	B	3236	HTL	C5A-C5-C4	-7.03	110.52	128.17
5	B	3236	HTL	C5A-C5-S1	-6.88	104.53	119.29
5	A	2236	HTL	C5A-C5-C4	-5.92	113.32	128.17
5	B	3236	HTL	O5G-C5B-C5A	5.68	131.45	108.63
5	A	2236	HTL	C5B-C5A-C5	-4.49	98.64	112.73
5	A	2236	HTL	C4-C5-S1	-4.40	106.01	110.56
5	A	2236	HTL	O5G-C5B-C5A	4.33	126.04	108.63
5	B	3236	HTL	C2A-C2'-N1'	4.11	121.58	117.20
5	A	2236	HTL	O2'-C1'-C2	4.01	122.89	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2236	HTL	C2A-C2'-N1'	3.93	121.39	117.20
5	B	3236	HTL	C4-C5-S1	-3.92	106.50	110.56
5	B	3236	HTL	C3'-C1'-C2	3.90	122.11	118.17
5	B	3236	HTL	C5B-C5A-C5	-3.49	101.79	112.73
5	A	2236	HTL	C4A-C4-C5	-3.33	119.23	127.75
5	A	2236	HTL	C35-N3-C4	-3.23	118.56	123.95
5	B	3236	HTL	C35-N3-C4	-3.04	118.87	123.95
5	B	3236	HTL	O22-P2-O21	2.89	122.10	110.83
5	A	2236	HTL	O22-P2-O21	2.87	122.01	110.83
5	B	3236	HTL	N1'-C2'-N3'	-2.87	120.76	125.53
5	A	2236	HTL	N1'-C2'-N3'	-2.76	120.94	125.53
5	B	3236	HTL	P1-O5G-C5B	2.47	133.02	121.26
5	A	2236	HTL	P1-O5G-C5B	2.26	132.02	121.26

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2236	HTL	O2'-C1'-C2-S1
5	A	2236	HTL	C3'-C1'-C2-S1
5	A	2236	HTL	P1-O11-P2-O23
5	B	3236	HTL	O2'-C1'-C2-S1
5	B	3236	HTL	S1-C5-C5A-C5B
5	A	2236	HTL	S1-C5-C5A-C5B
5	B	3236	HTL	P1-O11-P2-O23
5	B	3236	HTL	C5'-C35-N3-C2
5	A	2236	HTL	C5-C5A-C5B-O5G
5	B	3236	HTL	P1-O11-P2-O21
5	B	3236	HTL	C3'-C1'-C2-S1
5	A	2236	HTL	P1-O11-P2-O21

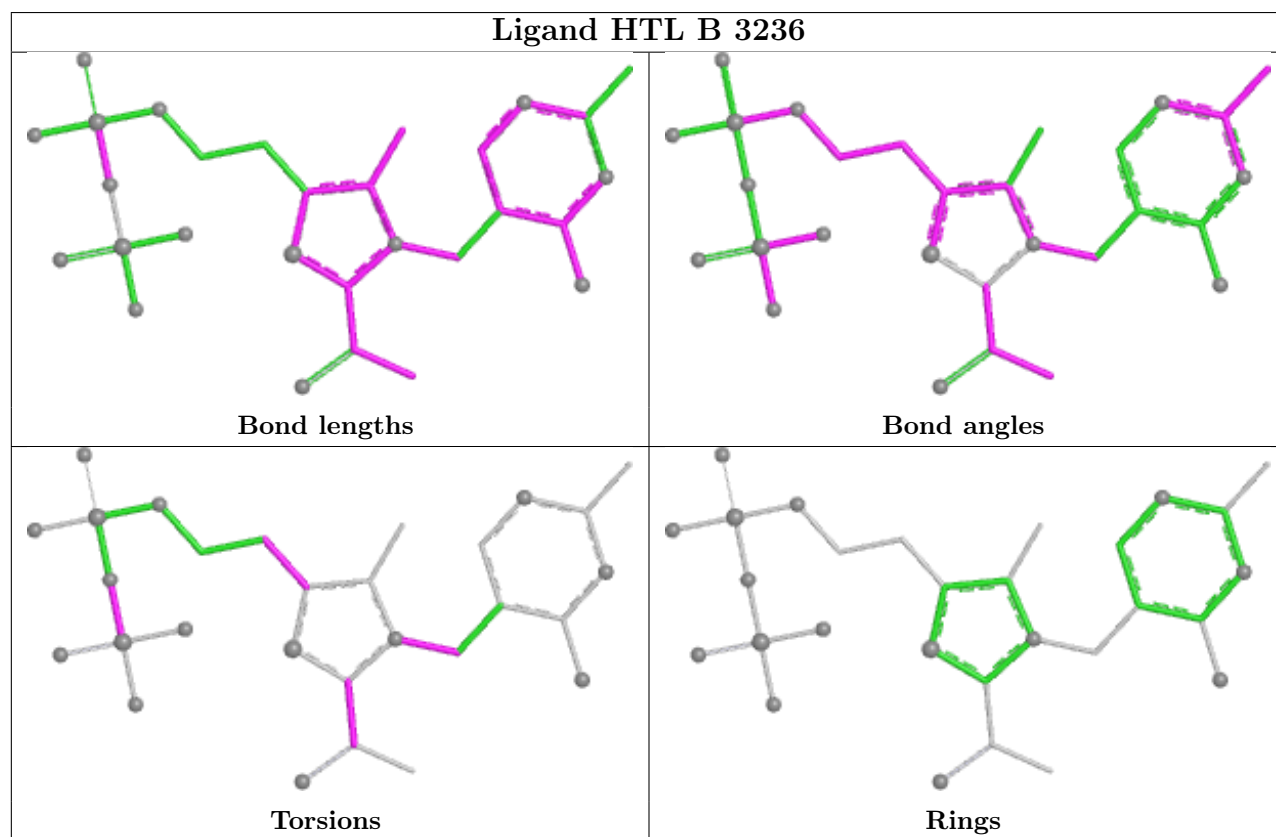
There are no ring outliers.

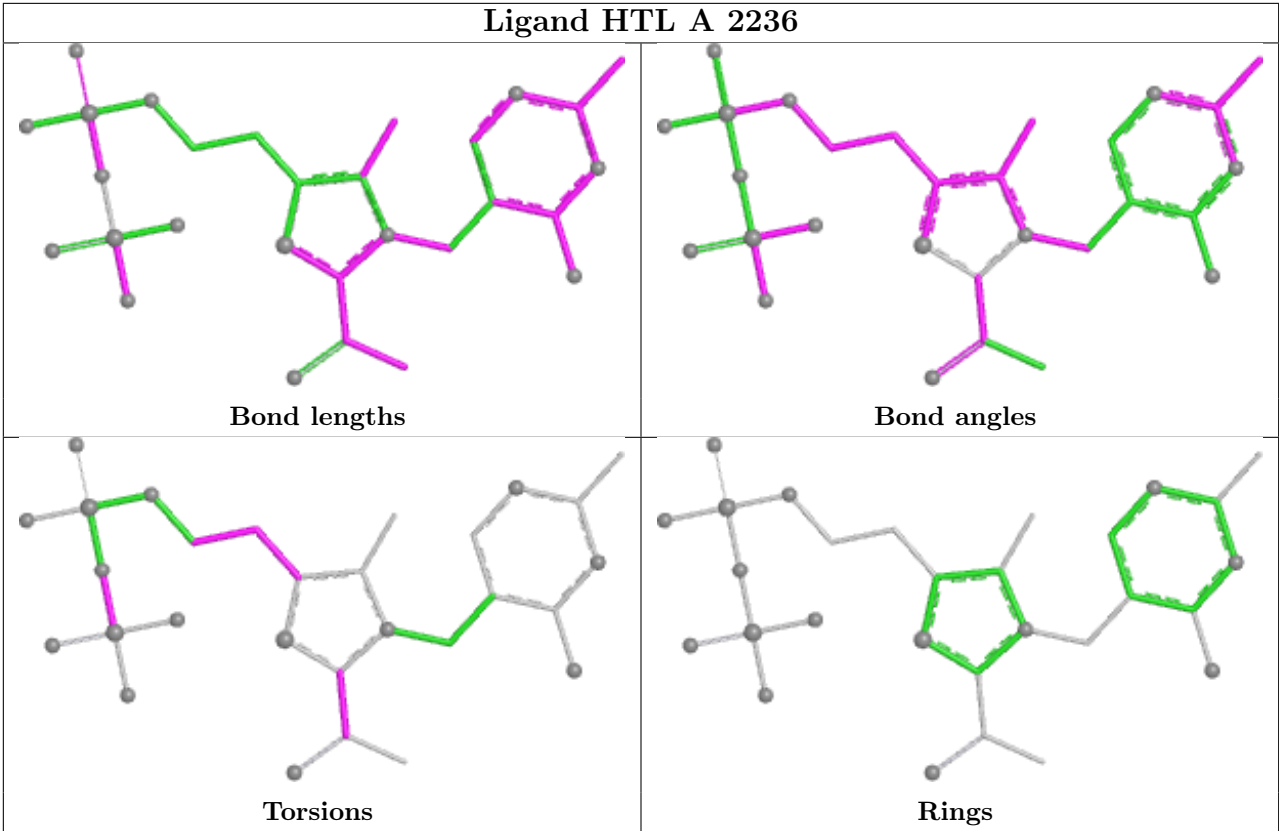
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3236	HTL	2	0
5	A	2236	HTL	3	0
6	A	2240	CO2	1	0
6	B	3240	CO2	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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1231:LYS	C	1232:LYS	N	2.00

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.