Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 09:22 AM EDT

PDB ID	:	1KEK
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:

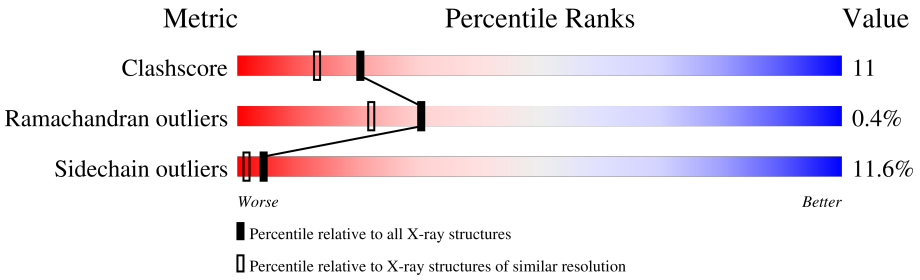
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1231	70% 23% 5% ·
1	B	1231	73% 21% · ·

2 Entry composition (i)

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			

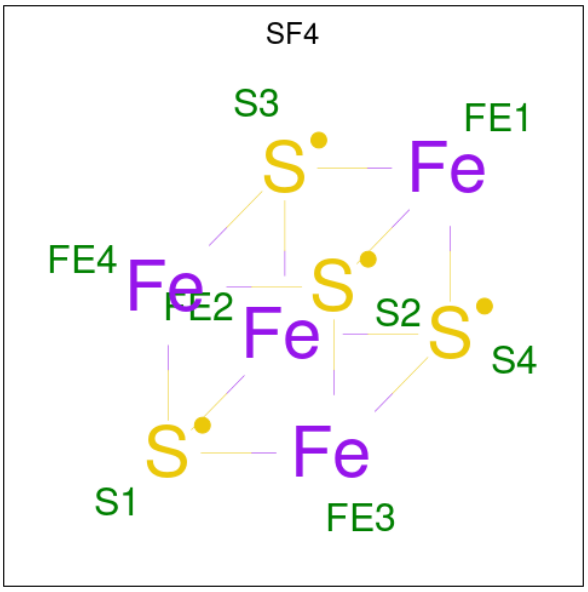
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: CA) (formula: Ca).

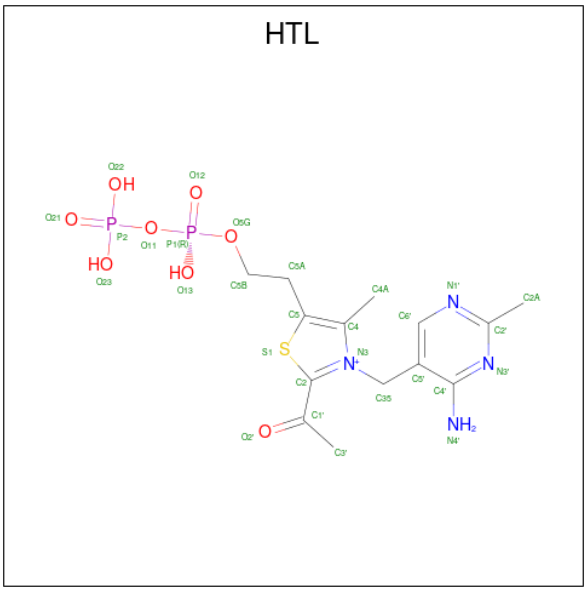
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



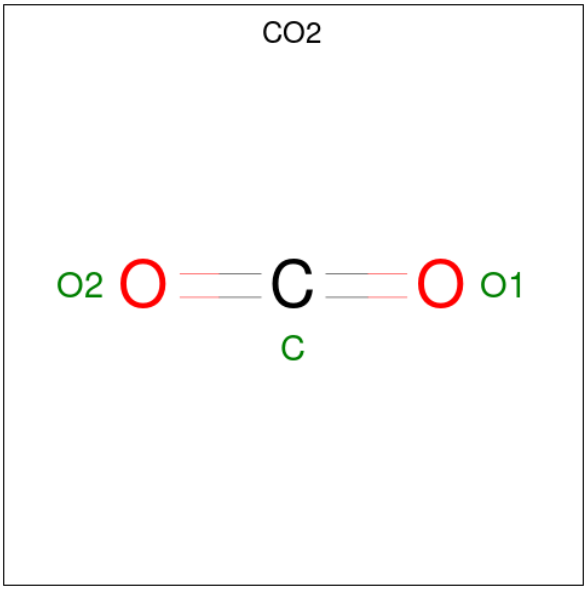
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0
4	A	1	Total Fe S 8 4 4	0	0
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0

- Molecule 5 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: 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 (three-letter code: CO2) (formula: CO_2).



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 O 851 851	0	0
7	B	1042	Total O 1042 1042	0	0

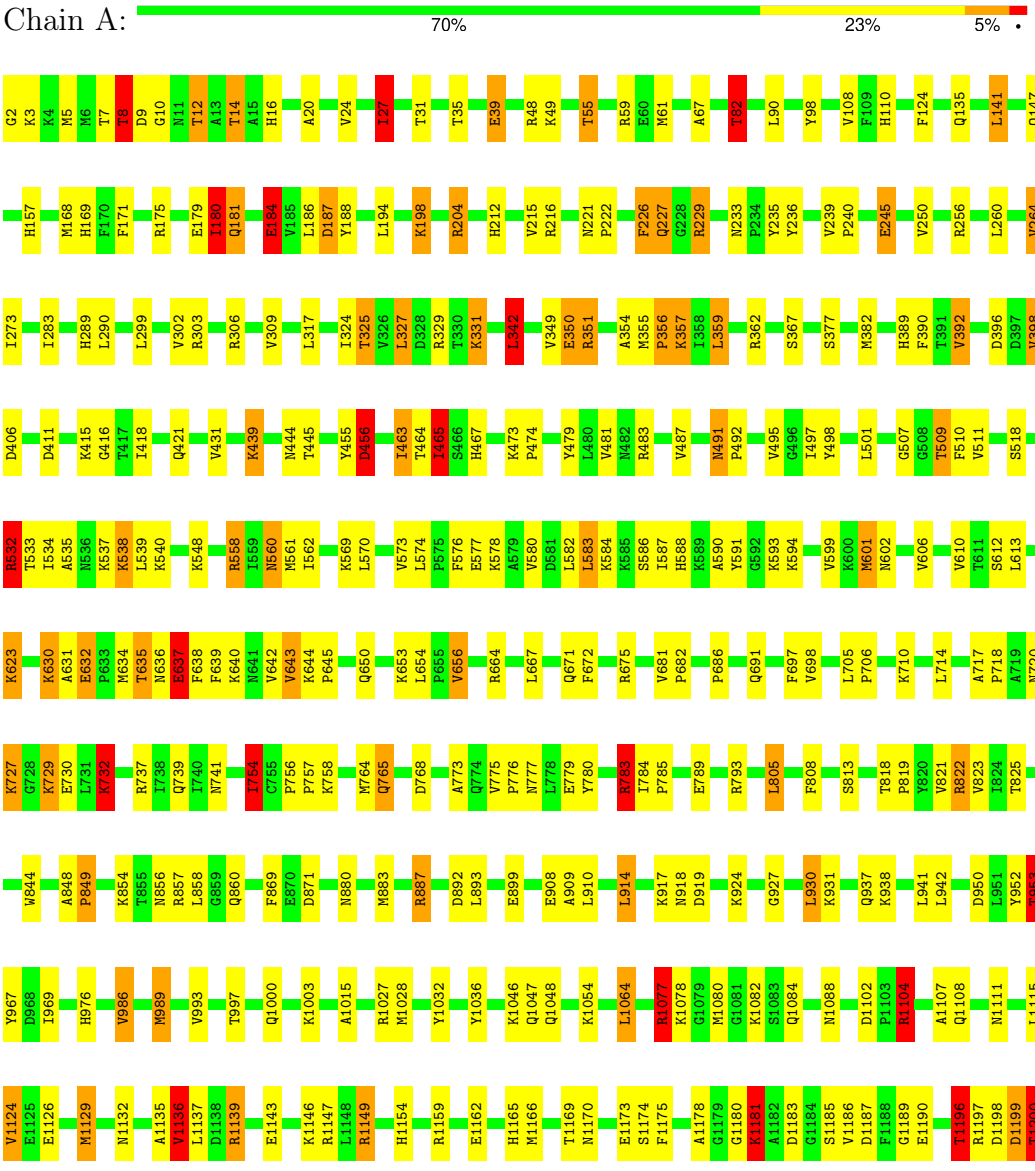
3 Residue-property plots (i)

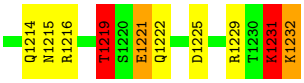
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

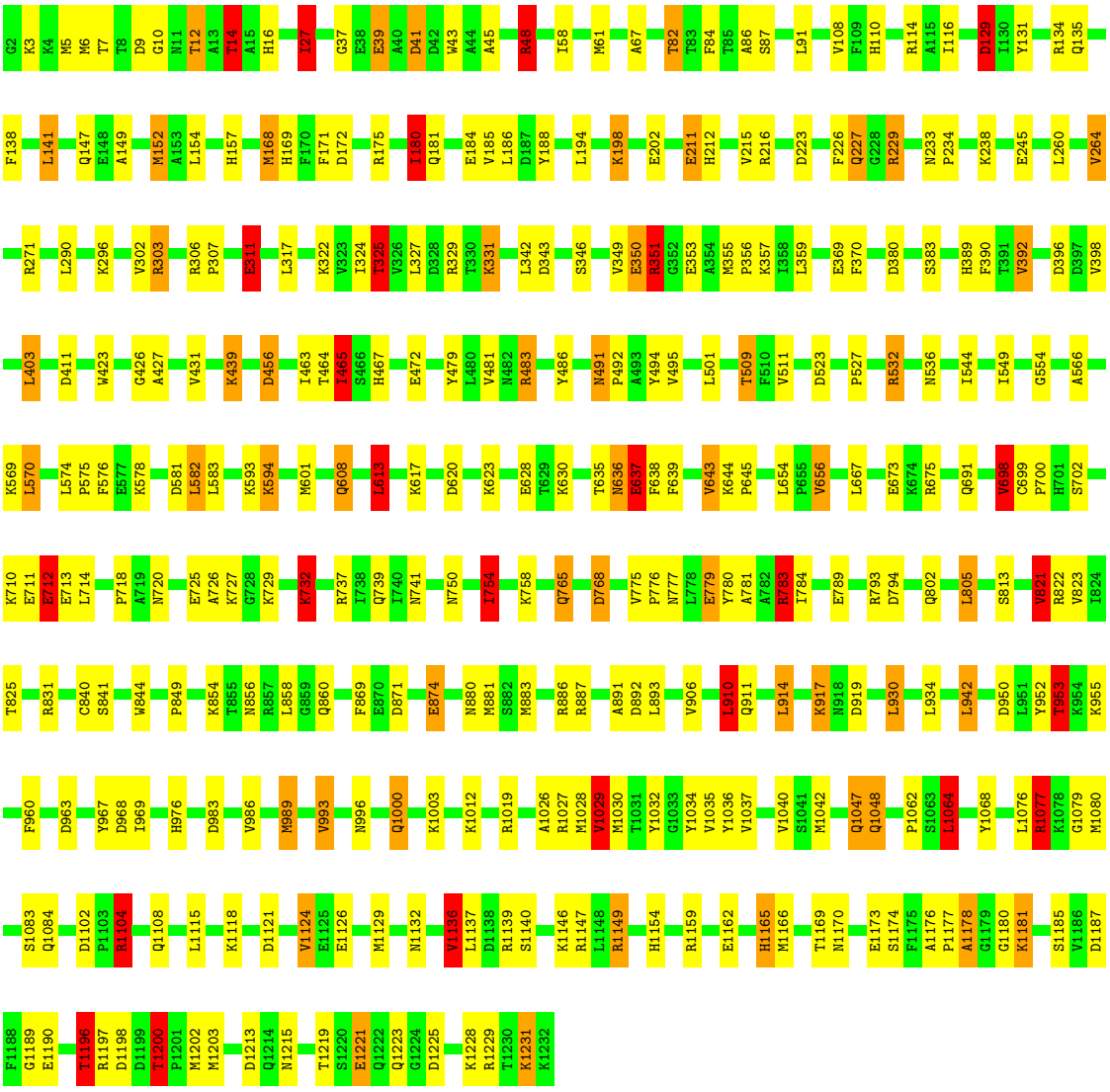
Chain A:





• Molecule 1: Pyruvate-Ferredoxin Oxidoreductase

Chain B:



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HTL, CA, MG, SF4, 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	0.78	10/9585 (0.1%)	1.56	147/12954 (1.1%)
1	B	1.07	14/9585 (0.1%)	1.63	154/12954 (1.2%)
All	All	0.94	24/19170 (0.1%)	1.60	301/25908 (1.2%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	732	LYS	CD-CE	56.96	2.93	1.51
1	B	1231	LYS	C-N	28.83	2.00	1.34
1	B	732	LYS	CG-CD	-20.40	0.83	1.52
1	A	601	MET	C-O	-15.37	0.94	1.23
1	B	711	GLU	C-O	-15.06	0.94	1.23
1	A	601	MET	CA-CB	-14.13	1.22	1.53
1	A	601	MET	CA-C	14.07	1.89	1.52
1	B	712	GLU	C-O	-13.72	0.97	1.23
1	B	711	GLU	CA-CB	-12.56	1.26	1.53
1	A	532	ARG	CA-C	11.83	1.83	1.52
1	B	732	LYS	CA-CB	-10.97	1.29	1.53
1	B	712	GLU	CA-C	10.27	1.79	1.52
1	A	1147	ARG	CG-CD	9.54	1.75	1.51
1	B	712	GLU	CA-CB	-9.17	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	908	GLU	CB-CG	-9.12	1.34	1.52
1	B	1126	GLU	C-O	-9.12	1.06	1.23
1	A	532	ARG	CA-CB	-7.74	1.36	1.53
1	B	711	GLU	CA-C	7.53	1.72	1.52
1	B	48	ARG	CD-NE	-7.51	1.33	1.46
1	A	637	GLU	CA-CB	5.64	1.66	1.53
1	A	532	ARG	C-N	-5.56	1.21	1.34
1	A	540	LYS	CD-CE	-5.39	1.37	1.51
1	B	245	GLU	C-O	-5.22	1.13	1.23
1	B	637	GLU	CD-OE2	5.10	1.31	1.25

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	532	ARG	CD-NE-CZ	35.55	173.37	123.60
1	B	48	ARG	CD-NE-CZ	30.27	165.97	123.60
1	A	204	ARG	CD-NE-CZ	29.99	165.58	123.60
1	A	48	ARG	NE-CZ-NH2	-21.39	109.60	120.30
1	A	351	ARG	NE-CZ-NH1	21.10	130.85	120.30
1	B	732	LYS	CG-CD-CE	-20.30	51.01	111.90
1	A	601	MET	O-C-N	19.00	153.10	122.70
1	A	351	ARG	NE-CZ-NH2	-17.44	111.58	120.30
1	B	732	LYS	N-CA-CB	17.03	141.25	110.60
1	A	204	ARG	NE-CZ-NH1	-15.41	112.59	120.30
1	B	1077	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	B	48	ARG	CG-CD-NE	14.70	142.67	111.80
1	A	48	ARG	CD-NE-CZ	14.58	144.01	123.60
1	B	351	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	B	306	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	B	48	ARG	NE-CZ-NH2	-14.07	113.26	120.30
1	B	712	GLU	N-CA-CB	13.68	135.22	110.60
1	A	601	MET	N-CA-CB	13.55	135.00	110.60
1	B	1231	LYS	CA-C-N	-13.40	87.72	117.20
1	A	664	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	A	1205	ARG	NE-CZ-NH1	-12.02	114.29	120.30
1	B	822	ARG	NE-CZ-NH1	-11.73	114.43	120.30
1	B	1147	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	B	355	MET	CA-CB-CG	11.64	133.09	113.30
1	A	1104	ARG	NE-CZ-NH2	11.58	126.09	120.30
1	A	532	ARG	O-C-N	11.37	140.90	122.70
1	B	793	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	A	1104	ARG	NE-CZ-NH1	-11.17	114.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	48	ARG	NH1-CZ-NH2	11.05	131.55	119.40
1	A	1200	THR	N-CA-CB	-10.95	89.49	110.30
1	A	216	ARG	CD-NE-CZ	10.89	138.85	123.60
1	B	1159	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	B	1104	ARG	CD-NE-CZ	10.79	138.71	123.60
1	A	783	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	712	GLU	O-C-N	10.65	139.75	122.70
1	A	887	ARG	NE-CZ-NH2	10.54	125.57	120.30
1	A	832	MET	CA-CB-CG	10.32	130.84	113.30
1	B	48	ARG	NE-CZ-NH1	-10.28	115.16	120.30
1	A	351	ARG	CD-NE-CZ	10.27	137.98	123.60
1	B	675	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	919	ASP	CB-CG-OD1	9.88	127.19	118.30
1	B	351	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	A	601	MET	CA-C-N	-9.69	95.88	117.20
1	A	1149	ARG	NE-CZ-NH2	-9.67	115.46	120.30
1	B	456	ASP	CB-CG-OD1	9.67	127.00	118.30
1	A	1205	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	A	1104	ARG	CD-NE-CZ	9.61	137.05	123.60
1	A	675	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	B	675	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	B	380	ASP	CB-CG-OD1	9.23	126.61	118.30
1	A	675	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	B	711	GLU	N-CA-CB	9.13	127.03	110.60
1	B	532	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	A	48	ARG	NH1-CZ-NH2	8.93	129.23	119.40
1	B	822	ARG	NE-CZ-NH2	8.93	124.77	120.30
1	B	1136	VAL	CB-CA-C	-8.90	94.48	111.40
1	A	27	ILE	CA-CB-CG2	8.84	128.57	110.90
1	B	1032	TYR	CB-CG-CD2	8.83	126.30	121.00
1	B	172	ASP	CB-CG-OD2	8.81	126.23	118.30
1	A	1136	VAL	CB-CA-C	-8.73	94.82	111.40
1	A	908	GLU	CA-CB-CG	8.71	132.55	113.40
1	A	675	ARG	CD-NE-CZ	8.66	135.72	123.60
1	A	306	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	A	1124	VAL	CB-CA-C	-8.46	95.32	111.40
1	A	1196	THR	N-CA-CB	-8.36	94.41	110.30
1	B	216	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	39	GLU	OE1-CD-OE2	8.34	133.30	123.30
1	B	131	TYR	CB-CG-CD1	-8.31	116.01	121.00
1	A	1219	THR	N-CA-CB	-8.30	94.53	110.30
1	B	392	VAL	CB-CA-C	-8.27	95.68	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	455	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	B	1221	GLU	CA-CB-CG	8.17	131.38	113.40
1	B	1036	TYR	CB-CG-CD1	8.15	125.89	121.00
1	B	82	THR	CB-CA-C	-8.11	89.71	111.60
1	A	532	ARG	CA-C-O	-8.11	103.08	120.10
1	B	989	MET	CG-SD-CE	-8.04	87.33	100.20
1	B	712	GLU	CA-C-N	-7.98	99.64	117.20
1	B	732	LYS	CB-CA-C	-7.96	94.49	110.40
1	B	27	ILE	CA-CB-CG2	7.94	126.78	110.90
1	B	711	GLU	CA-C-N	-7.93	99.76	117.20
1	B	675	ARG	CD-NE-CZ	7.84	134.57	123.60
1	B	711	GLU	O-C-N	7.82	135.21	122.70
1	B	343	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	B	175	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	A	256	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	1126	GLU	N-CA-CB	7.67	124.40	110.60
1	B	1200	THR	N-CA-CB	-7.66	95.75	110.30
1	A	783	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	369	GLU	OE1-CD-OE2	7.55	132.36	123.30
1	A	8	THR	N-CA-CB	7.54	124.62	110.30
1	B	698	VAL	N-CA-CB	-7.54	94.92	111.50
1	A	392	VAL	CB-CA-C	-7.53	97.10	111.40
1	B	1165	HIS	N-CA-CB	7.51	124.12	110.60
1	A	1104	ARG	CG-CD-NE	-7.48	96.09	111.80
1	A	887	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	A	857	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	350	GLU	OE1-CD-OE2	7.34	132.11	123.30
1	A	857	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	455	TYR	CB-CG-CD1	7.30	125.38	121.00
1	B	952	TYR	CB-CG-CD1	-7.27	116.64	121.00
1	B	1196	THR	N-CA-CB	-7.22	96.58	110.30
1	A	1165	HIS	N-CA-CB	7.21	123.59	110.60
1	B	1032	TYR	CB-CG-CD1	-7.21	116.67	121.00
1	B	114	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	180	ILE	CA-CB-CG2	7.14	125.17	110.90
1	B	331	LYS	CD-CE-NZ	-7.13	95.30	111.70
1	A	479	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	A	59	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	A	1129	MET	CG-SD-CE	7.10	111.57	100.20
1	B	129	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	187	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	B	39	GLU	OE1-CD-OE2	7.05	131.76	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	LYS	CA-CB-CG	7.00	128.80	113.40
1	B	41	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	B	968	ASP	CB-CG-OD2	6.95	124.56	118.30
1	A	82	THR	CB-CA-C	-6.94	92.85	111.60
1	B	1104	ARG	CG-CD-NE	-6.91	97.28	111.80
1	B	325	THR	N-CA-CB	6.90	123.41	110.30
1	A	914	LEU	CA-CB-CG	6.89	131.14	115.30
1	A	39	GLU	CG-CD-OE2	-6.87	104.56	118.30
1	A	264	VAL	CA-CB-CG1	6.79	121.08	110.90
1	B	698	VAL	CG1-CB-CG2	6.78	121.75	110.90
1	A	306	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	952	TYR	CB-CG-CD2	6.70	125.02	121.00
1	A	39	GLU	CA-CB-CG	-6.66	98.75	113.40
1	A	637	GLU	CA-CB-CG	6.64	128.02	113.40
1	B	306	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	1139	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	793	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	532	ARG	N-CA-CB	6.62	122.52	110.60
1	B	523	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	152	MET	CG-SD-CE	-6.56	89.70	100.20
1	B	1077	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	168	MET	CG-SD-CE	6.48	110.56	100.20
1	A	302	VAL	CA-CB-CG2	6.47	120.61	110.90
1	A	871	ASP	CB-CG-OD2	6.47	124.13	118.30
1	B	783	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	B	370	PHE	CB-CG-CD1	-6.45	116.29	120.80
1	B	967	TYR	CB-CG-CD1	6.38	124.83	121.00
1	B	914	LEU	CA-CB-CG	6.37	129.95	115.30
1	B	823	VAL	CA-CB-CG2	6.37	120.45	110.90
1	A	656	VAL	CA-CB-CG2	6.33	120.40	110.90
1	A	1197	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	98	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	A	793	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	B	483	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	B	86	ALA	CB-CA-C	-6.27	100.70	110.10
1	B	27	ILE	N-CA-CB	-6.26	96.41	110.80
1	B	1136	VAL	N-CA-CB	6.25	125.25	111.50
1	B	1029	VAL	CA-CB-CG2	6.25	120.27	110.90
1	A	822	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	B	479	TYR	CB-CG-CD1	-6.25	117.25	121.00
1	A	226	PHE	CB-CG-CD1	-6.24	116.44	120.80
1	B	919	ASP	CB-CG-OD1	6.24	123.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	392	VAL	N-CA-CB	6.22	125.19	111.50
1	A	601	MET	C-N-CA	-6.22	106.15	121.70
1	A	558	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	A	823	VAL	CA-CB-CG2	6.13	120.09	110.90
1	A	848	ALA	CA-C-O	-6.12	107.25	120.10
1	A	532	ARG	C-N-CA	-6.12	106.40	121.70
1	B	613	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	521	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	465	ILE	CB-CA-C	6.09	123.78	111.60
1	B	1124	VAL	CB-CA-C	-6.09	99.83	111.40
1	A	141	LEU	CA-CB-CG	6.08	129.27	115.30
1	A	306	ARG	O-C-N	6.08	132.64	121.10
1	B	456	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	350	GLU	OE1-CD-OE2	6.07	130.58	123.30
1	B	983	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	486	TYR	CB-CG-CD2	6.04	124.62	121.00
1	A	55	THR	OG1-CB-CG2	-6.04	96.12	110.00
1	B	1027	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	306	ARG	CA-C-O	-6.00	107.51	120.10
1	B	768	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	1034	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	A	456	ASP	CB-CA-C	-5.98	98.44	110.40
1	A	664	ARG	NH1-CZ-NH2	5.98	125.98	119.40
1	B	229	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	967	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	235	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	1036	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	B	264	VAL	N-CA-CB	-5.96	98.39	111.50
1	A	1077	ARG	CD-NE-CZ	5.95	131.93	123.60
1	B	303	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	B	465	ILE	CA-CB-CG2	5.92	122.74	110.90
1	B	636	ASN	CA-CB-CG	-5.90	100.42	113.40
1	A	456	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	1027	ARG	CD-NE-CZ	5.89	131.84	123.60
1	A	184	GLU	CA-CB-CG	5.86	126.30	113.40
1	A	1077	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	1136	VAL	CG1-CB-CG2	5.82	120.21	110.90
1	A	1149	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	82	THR	N-CA-CB	5.79	121.30	110.30
1	A	303	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	754	ILE	CA-CB-CG2	5.78	122.46	110.90
1	B	456	ASP	CB-CA-C	-5.77	98.85	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	993	VAL	N-CA-CB	-5.75	98.84	111.50
1	B	138	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	B	271	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	1216	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	B	608	GLN	CA-CB-CG	5.72	125.99	113.40
1	A	204	ARG	NH1-CZ-NH2	5.71	125.69	119.40
1	A	793	ARG	CG-CD-NE	-5.71	99.81	111.80
1	B	1149	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	154	LEU	CB-CG-CD2	5.69	120.68	111.00
1	A	82	THR	N-CA-CB	5.68	121.10	110.30
1	B	953	THR	CA-CB-OG1	5.67	120.90	109.00
1	A	532	ARG	CA-C-N	-5.65	104.77	117.20
1	B	6	MET	CA-CB-CG	5.64	122.89	113.30
1	B	180	ILE	CA-CB-CG2	5.63	122.16	110.90
1	B	821	VAL	N-CA-CB	5.63	123.88	111.50
1	A	48	ARG	CB-CG-CD	-5.62	97.00	111.60
1	B	910	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	31	THR	CA-C-O	-5.58	108.37	120.10
1	A	406	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	27	ILE	N-CA-CB	-5.58	97.98	110.80
1	B	793	ARG	N-CA-CB	-5.58	100.56	110.60
1	B	392	VAL	CG1-CB-CG2	5.57	119.82	110.90
1	A	831	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	A	986	VAL	CA-CB-CG1	5.53	119.19	110.90
1	B	486	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	351	ARG	CG-CD-NE	5.51	123.36	111.80
1	B	1200	THR	CA-CB-CG2	5.49	120.08	112.40
1	A	1221	GLU	CA-CB-CG	5.48	125.45	113.40
1	A	1124	VAL	N-CA-CB	5.46	123.51	111.50
1	A	960	PHE	CB-CG-CD1	-5.45	116.99	120.80
1	A	1147	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A	175	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	479	TYR	CB-CG-CD2	5.42	124.25	121.00
1	B	245	GLU	O-C-N	-5.41	114.04	122.70
1	A	264	VAL	N-CA-CB	-5.41	99.60	111.50
1	B	264	VAL	CB-CA-C	5.41	121.68	111.40
1	A	329	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	342	LEU	CB-CG-CD1	5.40	120.18	111.00
1	B	1064	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	1108	GLN	CA-CB-CG	5.39	125.26	113.40
1	B	754	ILE	CA-CB-CG2	5.39	121.67	110.90
1	B	656	VAL	CA-CB-CG1	5.36	118.94	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	953	THR	CA-CB-OG1	5.35	120.23	109.00
1	B	821	VAL	CA-CB-CG2	5.35	118.92	110.90
1	A	356	PRO	CA-C-N	5.34	128.96	117.20
1	A	637	GLU	N-CA-CB	-5.33	101.00	110.60
1	A	698	VAL	N-CA-CB	-5.33	99.77	111.50
1	B	960	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	B	886	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	924	LYS	CD-CE-NZ	5.32	123.94	111.70
1	A	637	GLU	CA-C-O	-5.31	108.94	120.10
1	A	1027	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	B	311	GLU	CA-CB-CG	5.31	125.08	113.40
1	A	899	GLU	CA-CB-CG	5.30	125.06	113.40
1	A	1187	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	892	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	919	ASP	OD1-CG-OD2	-5.25	113.32	123.30
1	B	307	PRO	N-CA-CB	5.25	109.61	103.30
1	B	39	GLU	CA-CB-CG	-5.25	101.85	113.40
1	B	963	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	967	TYR	CB-CG-CD1	5.25	124.15	121.00
1	A	236	TYR	CD1-CG-CD2	5.24	123.66	117.90
1	A	986	VAL	CA-CB-CG2	5.24	118.75	110.90
1	A	479	TYR	CB-CG-CD2	5.24	124.14	121.00
1	A	245	GLU	CA-CB-CG	5.23	124.92	113.40
1	B	1047	GLN	CB-CG-CD	5.23	125.19	111.60
1	A	456	ASP	CB-CG-OD1	5.22	122.99	118.30
1	B	494	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	B	134	ARG	CG-CD-NE	5.20	122.73	111.80
1	B	712	GLU	C-N-CA	-5.20	108.70	121.70
1	B	581	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	1136	VAL	N-CA-CB	5.19	122.92	111.50
1	B	794	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	1121	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	223	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	392	VAL	CA-CB-CG2	5.18	118.67	110.90
1	B	329	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	1159	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	302	VAL	CA-CB-CG2	5.17	118.65	110.90
1	B	673	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	B	1068	TYR	CB-CG-CD2	5.14	124.09	121.00
1	A	399	THR	CA-CB-CG2	-5.14	105.21	112.40
1	A	952	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	637	GLU	CB-CA-C	-5.13	100.14	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	637	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	B	14	THR	CA-CB-OG1	5.13	119.77	109.00
1	B	1159	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	465	ILE	CA-CB-CG2	5.12	121.13	110.90
1	A	229	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	1213	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	236	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	A	1219	THR	OG1-CB-CG2	5.07	121.67	110.00
1	A	465	ILE	CB-CA-C	5.05	121.71	111.60
1	B	188	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	B	211	GLU	CG-CD-OE2	-5.04	108.22	118.30
1	B	1124	VAL	CG1-CB-CG2	5.04	118.96	110.90
1	A	1032	TYR	CG-CD2-CE2	-5.03	117.27	121.30
1	B	411	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	8	THR	CB-CA-C	-5.03	98.03	111.60
1	B	1068	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	B	911	GLN	CB-CG-CD	5.02	124.65	111.60
1	B	302	VAL	CA-CB-CG1	5.01	118.42	110.90
1	A	1199	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	B	307	PRO	CA-N-CD	-5.01	104.49	111.50
1	B	637	GLU	CB-CG-CD	5.00	127.71	114.20

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	237	0
1	B	9383	0	9261	203	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	37	0
7	B	1042	0	0	31	0
All	All	20775	0	18560	414	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 11.

All (414) 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: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: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:883:MET:HE3	1:A:887:ARG:HD2	1.58	0.83
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:B:883:MET:HE3	1:B:887:ARG:HD2	1.63	0.81
1:A:841:SER:HB3	1:A:989:MET:HE1	1.61	0.81
1:B:227:GLN:H	1:B:227:GLN:HE21	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:198:LYS:H	1:A:198:LYS:HZ3	1.35	0.72
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: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: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:A:1028:MET:HE2	1:B:1028:MET:HE2	1.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:B:7:THR:HB	1:B:180:ILE:HD11	1.79	0.62
1:B:883:MET:CE	1:B:887:ARG:HD2	2.29	0.62
1:B:10:GLY:O	1:B:14:THR:HG23	2.00	0.62
1:B:891:ALA:HB2	1:B:917:LYS:HZ1	1.64	0.62
1:A:8:THR:HG22	7:A:2981:HOH:O	1.99	0.62
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.35	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:B:5:MET:CE	1:B:184:GLU:HB2	2.32	0.60
1:A:416:GLY:C	7:A:3044:HOH:O	2.39	0.60
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: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:A:691:GLN:HE22	1:A:727:LYS:H	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:MET:HE1	1:B:184:GLU:HB2	1.84	0.58
1:B:883:MET:HE1	1:B:955:LYS:HG3	1.86	0.58
1:B:1187:ASP:HB3	1:B:1190:GLU:HG3	1.85	0.57
7:A:2421:HOH:O	1:B:953:THR:HG21	2.04	0.57
1:A:642:VAL:C	1:A:645:PRO:HD2	2.25	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:A:691:GLN:NE2	1:A:727:LYS:H	2.02	0.56
1:A:644:LYS:N	1:A:645:PRO:CD	2.68	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: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:B:821:VAL:HG12	1:B:989:MET:HE3	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:698:VAL:HG22	1:B:1084:GLN:CD	2.30	0.52
1:A:561:MET:HE1	1:A:583:LEU:HD22	1.92	0.52
1:B:779:GLU:C	1:B:783:ARG:HH11	2.13	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:351:ARG:HD3	1:B:353:GLU:HB2	1.92	0.51
1:B:135:GLN:H	1:B:135:GLN:NE2	2.09	0.51
1:A:1129:MET:CE	1:A:1149:ARG:HD3	2.41	0.51
1:B:390:PHE:CD1	1:B:403:LEU:HD22	2.46	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: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:989:MET:HE2	7:A:3079:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.24	0.50
1:A:630:LYS:C	1:A:632:GLU:H	2.14	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:A:1129:MET:HE2	1:A:1149:ARG:HD3	1.94	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: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:A:1129:MET:HE1	1:A:1135:ALA:HA	1.95	0.49
1:B:554:GLY:HA3	1:B:601:MET:HE2	1.94	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:B:883:MET:CE	1:B:955:LYS:HG3	2.42	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:221:ASN:HB3	1:A:222:PRO:CD	2.43	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: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
7:A:2373:HOH:O	1:B:1028:MET:HE3	2.14	0.48
1:A:473:LYS:HB3	1:A:474:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:1129:MET:CE	1:B:1149:ARG:HD3	2.44	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: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:1003:LYS:HZ3	1:B:976:HIS:HD2	1.63	0.46
1:A:390:PHE:CE1	1:A:403:LEU:HD22	2.51	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:350:GLU:CD	1:B:389:HIS:HE1	2.19	0.46
1:A:561:MET:HE1	1:A:583:LEU:CD2	2.45	0.46
1:B:554:GLY:HA3	1:B:601:MET:CE	2.46	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:5:MET:HE1	7:A:3054:HOH:O	2.15	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:B:891:ALA:CB	1:B:917:LYS:HZ1	2.29	0.46
1:A:198:LYS:HZ3	1:A:198:LYS:N	2.09	0.46
1:B:732:LYS:CD	1:B:732:LYS:CA	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:B:1129:MET:HE1	1:B:1149:ARG:HD3	1.98	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:578:LYS:HG2	1:B:582:LEU:HD22	1.98	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:B:1177:PRO:O	1:B:1178:ALA:HB2	2.17	0.44
1:A:389:HIS:HE1	1:B:350:GLU:CD	2.21	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:1180:GLY:H	1:A:1181:LYS:HZ1	1.65	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:576:PHE:O	1:A:580:VAL:HG23	2.18	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1199:ASP:CG	1:A:1214:GLN:HE22	2.21	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:B:779:GLU:C	1:B:783:ARG:NH1	2.72	0.43
1:B:821:VAL:CG1	1:B:989:MET:CE	2.96	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:A:180:ILE:HD12	1:A:181:GLN:N	2.34	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: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: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:B:821:VAL:CG1	1:B:989:MET:HE3	2.49	0.42
1:A:1200:THR:HG23	1:A:1202:MET:HE3	2.01	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:1028:MET:CE	1:B:1028:MET:HB3	2.49	0.42
1:B:141:LEU:HD13	1:B:152:MET:HB3	2.01	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:A:841:SER:HB3	1:A:989:MET:CE	2.42	0.42
1:B:574:LEU:HB3	1:B:575:PRO:HD2	2.02	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:650:GLN:CD	1:A:653:LYS:HE3	2.39	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:601:MET:HE1	7:B:3967:HOH:O	2.19	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:A:24:VAL:CG1	1:B:881:MET:HE1	2.50	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: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:24:VAL:HG13	1:B:881:MET:HE1	2.03	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:874:GLU:CD	7:B:4242:HOH:O	2.58	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:491:ASN:HA	1:A:492:PRO:HD2	1.83	0.40
1:A:764:MET:C	1:A:765:GLN:HG2	2.41	0.40
7:A:2543:HOH:O	1:B:1200:THR:HG21	2.20	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:A:730:GLU:CD	1:A:730:GLU:H	2.24	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:B:1076:LEU:HB3	7:B:4233:HOH:O	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%)	1181 (96%)	42 (3%)	6 (0%)	25	17
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	978/978 (100%)	856 (88%)	122 (12%)	3	1
1	B	978/978 (100%)	873 (89%)	105 (11%)	5	2
All	All	1956/1956 (100%)	1729 (88%)	227 (12%)	4	1

All (227) 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

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Mol	Chain	Res	Type
1	A	82	THR
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	226	PHE
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	317	LEU
1	A	324	ILE
1	A	325	THR
1	A	327	LEU
1	A	342	LEU
1	A	349	VAL
1	A	359	LEU
1	A	377	SER
1	A	392	VAL
1	A	398	VAL
1	A	403	LEU
1	A	415	LYS
1	A	439	LYS
1	A	456	ASP
1	A	463	ILE
1	A	465	ILE
1	A	491	ASN
1	A	495	VAL
1	A	501	LEU
1	A	509	THR
1	A	511	VAL
1	A	518	SER
1	A	524	LYS
1	A	532	ARG
1	A	538	LYS

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Mol	Chain	Res	Type
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	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	623	LYS
1	A	630	LYS
1	A	632	GLU
1	A	634	MET
1	A	635	THR
1	A	637	GLU
1	A	643	VAL
1	A	654	LEU
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	741	ASN
1	A	754	ILE
1	A	758	LYS
1	A	765	GLN
1	A	768	ASP
1	A	783	ARG
1	A	789	GLU
1	A	805	LEU
1	A	808	PHE
1	A	813	SER
1	A	831	ARG
1	A	849	PRO
1	A	858	LEU
1	A	880	ASN
1	A	893	LEU

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Mol	Chain	Res	Type
1	A	910	LEU
1	A	914	LEU
1	A	917	LYS
1	A	930	LEU
1	A	938	LYS
1	A	941	LEU
1	A	953	THR
1	A	989	MET
1	A	993	VAL
1	A	997	THR
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN
1	A	1064	LEU
1	A	1077	ARG
1	A	1082	LYS
1	A	1088	ASN
1	A	1104	ARG
1	A	1115	LEU
1	A	1124	VAL
1	A	1136	VAL
1	A	1137	LEU
1	A	1146	LYS
1	A	1170	ASN
1	A	1173	GLU
1	A	1181	LYS
1	A	1183	ASP
1	A	1196	THR
1	A	1200	THR
1	A	1219	THR
1	A	1225	ASP
1	A	1231	LYS
1	A	1232	LYS
1	B	12	THR
1	B	14	THR
1	B	27	ILE
1	B	48	ARG
1	B	82	THR
1	B	141	LEU
1	B	154	LEU
1	B	168	MET
1	B	180	ILE

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Mol	Chain	Res	Type
1	B	181	GLN
1	B	194	LEU
1	B	198	LYS
1	B	211	GLU
1	B	215	VAL
1	B	226	PHE
1	B	227	GLN
1	B	260	LEU
1	B	264	VAL
1	B	290	LEU
1	B	296	LYS
1	B	303	ARG
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	383	SER
1	B	392	VAL
1	B	403	LEU
1	B	439	LYS
1	B	465	ILE
1	B	472	GLU
1	B	483	ARG
1	B	491	ASN
1	B	501	LEU
1	B	509	THR
1	B	511	VAL
1	B	532	ARG
1	B	570	LEU
1	B	582	LEU
1	B	583	LEU
1	B	593	LYS
1	B	594	LYS
1	B	613	LEU
1	B	617	LYS
1	B	620	ASP
1	B	628	GLU

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Mol	Chain	Res	Type
1	B	630	LYS
1	B	637	GLU
1	B	643	VAL
1	B	654	LEU
1	B	698	VAL
1	B	702	SER
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
1	B	765	GLN
1	B	768	ASP
1	B	779	GLU
1	B	783	ARG
1	B	789	GLU
1	B	805	LEU
1	B	813	SER
1	B	821	VAL
1	B	831	ARG
1	B	858	LEU
1	B	874	GLU
1	B	880	ASN
1	B	893	LEU
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	993	VAL
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1064	LEU
1	B	1077	ARG
1	B	1104	ARG
1	B	1115	LEU

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	46	GLN
1	A	110	HIS
1	A	128	GLN
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	221	ASN
1	A	227	GLN
1	A	233	ASN
1	A	289	HIS
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	491	ASN
1	A	513	ASN
1	A	560	ASN
1	A	588	HIS
1	A	602	ASN
1	A	688	ASN

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Mol	Chain	Res	Type
1	A	691	GLN
1	A	693	ASN
1	A	720	ASN
1	A	739	GLN
1	A	741	ASN
1	A	750	ASN
1	A	765	GLN
1	A	774	GLN
1	A	777	ASN
1	A	836	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	1048	GLN
1	A	1084	GLN
1	A	1088	ASN
1	A	1132	ASN
1	A	1154	HIS
1	A	1215	ASN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	110	HIS
1	B	128	GLN
1	B	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	491	ASN

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Mol	Chain	Res	Type
1	B	513	ASN
1	B	536	ASN
1	B	560	ASN
1	B	602	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	765	GLN
1	B	774	GLN
1	B	777	ASN
1	B	836	ASN
1	B	860	GLN
1	B	866	ASN
1	B	880	ASN
1	B	911	GLN
1	B	918	ASN
1	B	976	HIS
1	B	1000	GLN
1	B	1048	GLN
1	B	1084	GLN
1	B	1088	ASN
1	B	1108	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 (i)

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	$\#\|Z\| > 2$
5	HTL	A	2236	2	25,30,30	3.94	13 (52%)	32,45,45	2.15	8 (25%)
5	HTL	B	3236	2	25,30,30	4.08	10 (40%)	32,45,45	1.90	7 (21%)
6	CO2	B	3240	-	2,2,2	0.26	0	1,1,1	0.49	0
4	SF4	B	3234	1	0,12,12	-	-	-		
4	SF4	B	3235	1	0,12,12	-	-	-		
6	CO2	A	2240	-	2,2,2	0.32	0	1,1,1	0.49	0
4	SF4	A	2234	1	0,12,12	-	-	-		
4	SF4	A	2233	1	0,12,12	-	-	-		
4	SF4	B	3233	1	0,12,12	-	-	-		
4	SF4	A	2235	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
5	HTL	A	2236	2	-	4/16/21/21	0/2/2/2
4	SF4	B	3234	1	-	-	0/6/5/5
4	SF4	B	3235	1	-	-	0/6/5/5
4	SF4	A	2234	1	-	-	0/6/5/5
4	SF4	B	3233	1	-	-	0/6/5/5
4	SF4	A	2233	1	-	-	0/6/5/5
5	HTL	B	3236	2	-	2/16/21/21	0/2/2/2
4	SF4	A	2235	1	-	-	0/6/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3236	HTL	C4'-N3'	11.10	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2236	HTL	C4'-N3'	9.02	1.47	1.35
5	A	2236	HTL	C2'-N1'	8.59	1.47	1.34
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	-8.00	1.33	1.49
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	B	3236	HTL	C5-S1	-4.97	1.64	1.74
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	A	2236	HTL	C4'-N4'	4.46	1.45	1.34
5	B	3236	HTL	C4-N3	-4.39	1.30	1.39
5	A	2236	HTL	C2A-C2'	-3.75	1.39	1.49
5	A	2236	HTL	C4A-C4	-3.30	1.42	1.49
5	A	2236	HTL	C3'-C1'	2.82	1.57	1.49
5	A	2236	HTL	C5A-C5	2.77	1.52	1.51
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	P1-O11	-2.25	1.57	1.59
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 (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2236	HTL	C4A-C4-N3	7.10	131.63	122.69
5	B	3236	HTL	C5A-C5-C4	-5.31	110.52	127.05
5	A	2236	HTL	C5A-C5-C4	-4.41	113.32	127.05
5	B	3236	HTL	C4-N3-C2	-4.35	106.21	108.64
5	B	3236	HTL	C2A-C2'-N1'	4.11	121.58	117.20
5	A	2236	HTL	C2A-C2'-N1'	3.93	121.39	117.20
5	A	2236	HTL	C4A-C4-C5	-3.83	119.23	127.60
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	C5-C4-N3	2.75	113.41	107.66
5	A	2236	HTL	C4-N3-C2	2.68	110.13	108.64
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 (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2236	HTL	C4-C5-C5A-C5B
5	A	2236	HTL	C5-C5A-C5B-O5G
5	A	2236	HTL	P1-O11-P2-O23
5	B	3236	HTL	P1-O11-P2-O23
5	B	3236	HTL	P1-O11-P2-O21
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	A	2236	HTL	3	0
5	B	3236	HTL	2	0
6	B	3240	CO2	1	0
6	A	2240	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 then 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.

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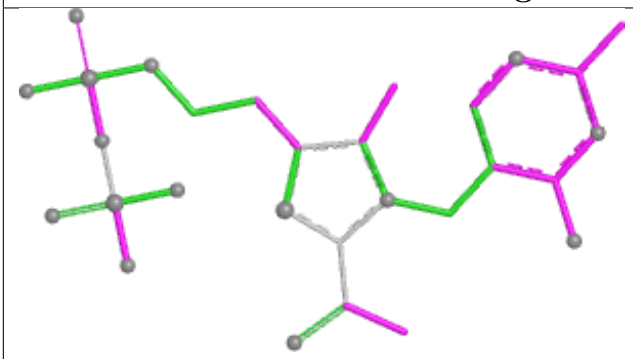
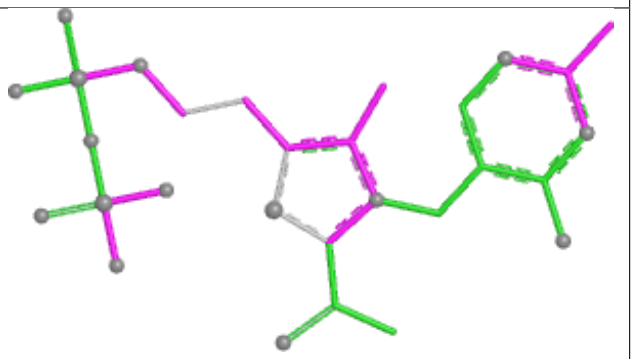
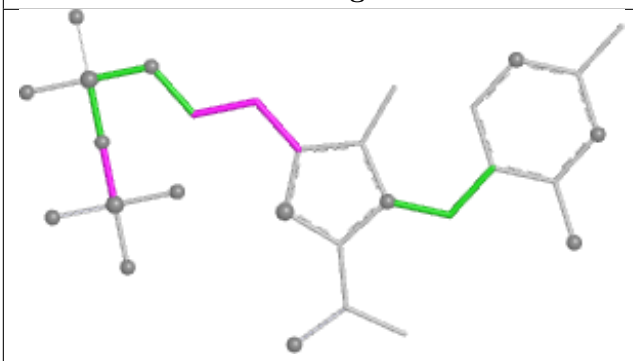


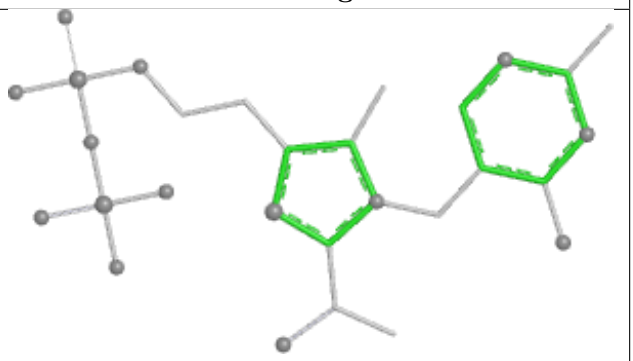
Bond lengths



Bond angles

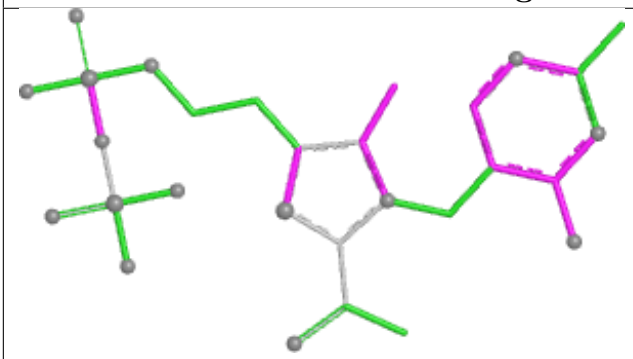


Torsions

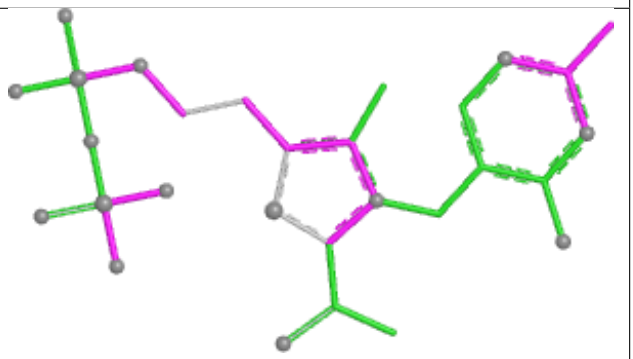


Rings

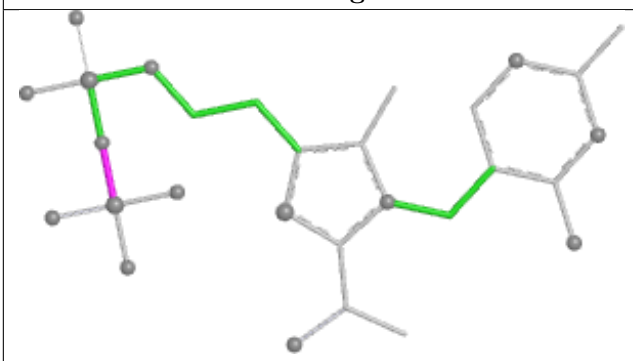
Ligand HTL B 3236



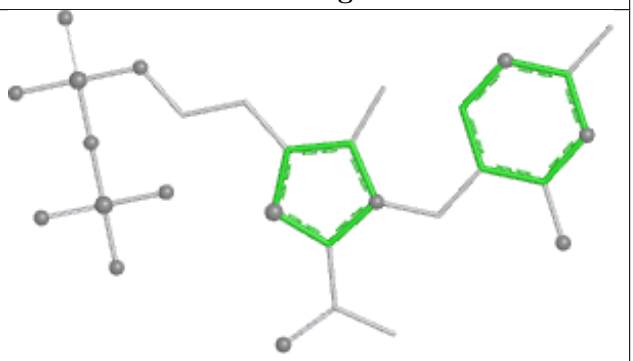
Bond lengths



Bond angles



Torsions



Rings

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.