Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 09:02 AM EDT

PDB ID	:	1B6S
Title	:	STRUCTURE OF N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE
Authors	:	Thoden, J.B.; Kappock, T.J.; Stubbe, J.; Holden, H.M.
Deposited on	:	1999-01-18
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

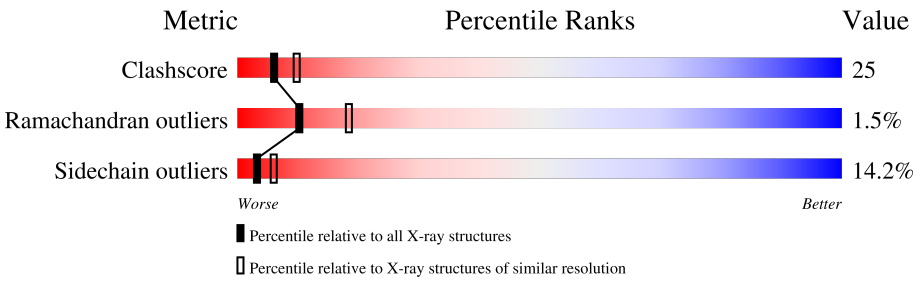
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	355	46% 41% 10% ••
1	B	355	50% 38% 12% •
1	C	355	46% 37% 13% • •
1	D	355	49% 38% 11% ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2751	1752	487	501	11	0	0	0
1	B	355	2784	1772	493	508	11	0	0	0
1	C	350	2747	1750	486	500	11	0	0	0
1	D	350	2747	1750	486	500	11	0	0	0

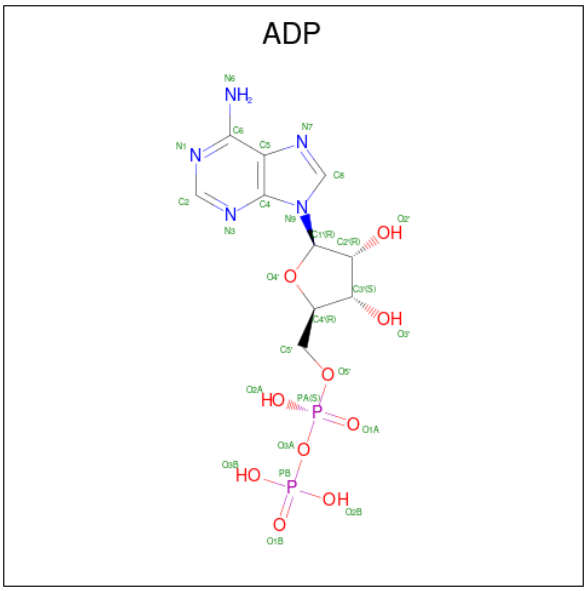
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ARG	GLN	conflict	UNP P09029
B	205	ARG	GLN	conflict	UNP P09029
C	205	ARG	GLN	conflict	UNP P09029
D	205	ARG	GLN	conflict	UNP P09029

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

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total	O	0	0
			107	107		
4	B	121	Total	O	0	0
			121	121		
4	C	136	Total	O	0	0
			136	136		
4	D	127	Total	O	0	0
			127	127		

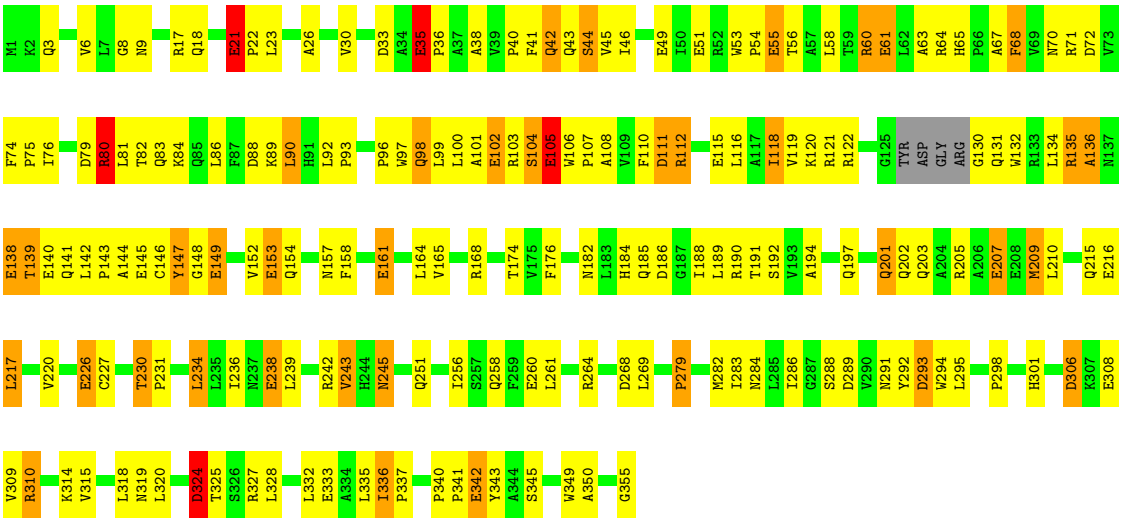
3 Residue-property plots (i)

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.

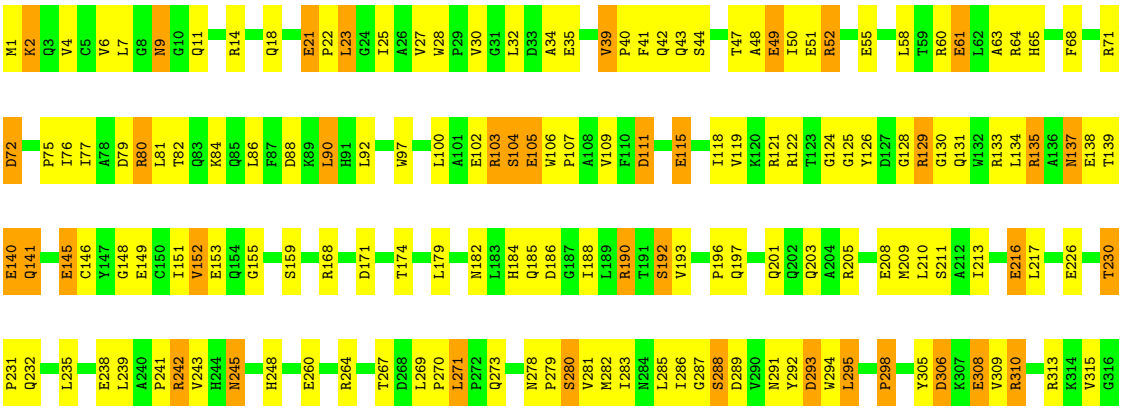
• Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)

Chain A: 46% 41% 10% ••



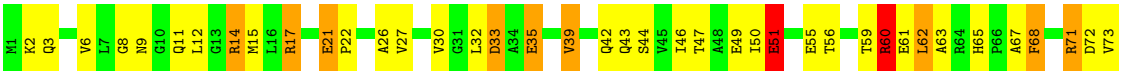
• Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)

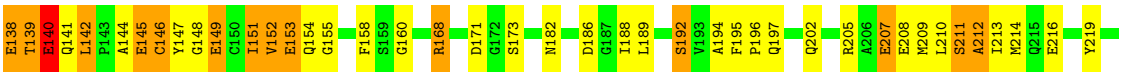
Chain B: 50% 38% 12% •

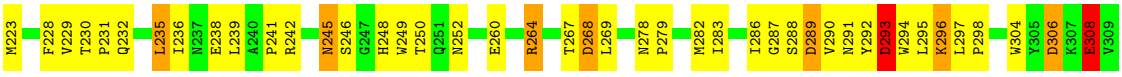


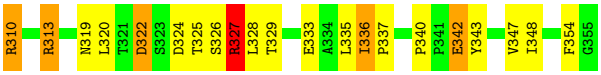
• Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)

Chain C:



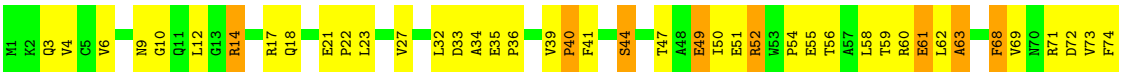


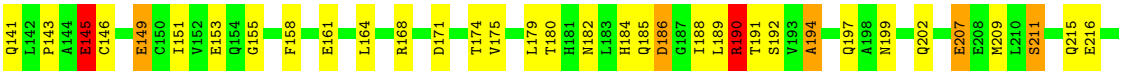


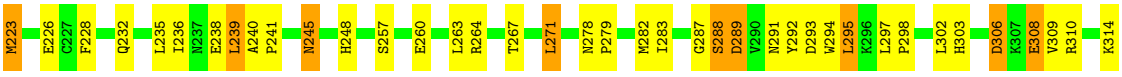


• Molecule 1: PROTEIN (N5-CARBOXYAMINOIMIDAZOLE RIBONUCLEOTIDE SYNTHETASE)

Chain D:







4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.60Å 92.10Å 102.60Å 66.10° 82.70° 81.80°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	95.7 (30.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.72	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11632	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	1.01	24/2819 (0.9%)	1.34	28/3841 (0.7%)
1	B	1.00	18/2853 (0.6%)	1.31	24/3888 (0.6%)
1	C	0.99	18/2815 (0.6%)	1.40	40/3836 (1.0%)
1	D	0.98	19/2815 (0.7%)	1.37	31/3836 (0.8%)
All	All	1.00	79/11302 (0.7%)	1.35	123/15401 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	ASP	CG-OD1	10.12	1.48	1.25
1	A	324	ASP	C-O	-9.72	1.04	1.23
1	B	260	GLU	CD-OE1	9.49	1.36	1.25
1	D	102	GLU	CD-OE1	9.12	1.35	1.25
1	B	65	HIS	CG-CD2	-8.89	1.20	1.35
1	A	61	GLU	CD-OE2	7.78	1.34	1.25
1	B	149	GLU	CD-OE2	7.59	1.33	1.25
1	D	140	GLU	CD-OE1	7.56	1.33	1.25
1	A	324	ASP	CA-C	7.47	1.72	1.52
1	D	260	GLU	CD-OE1	7.32	1.33	1.25
1	C	153	GLU	CD-OE1	7.21	1.33	1.25
1	C	260	GLU	CD-OE2	7.11	1.33	1.25
1	D	61	GLU	CD-OE2	7.07	1.33	1.25
1	B	61	GLU	CD-OE2	7.05	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	GLU	CD-OE1	6.90	1.33	1.25
1	A	35	GLU	CD-OE1	6.84	1.33	1.25
1	B	216	GLU	CD-OE1	6.84	1.33	1.25
1	D	216	GLU	CD-OE1	6.81	1.33	1.25
1	A	51	GLU	CD-OE2	6.81	1.33	1.25
1	C	35	GLU	CD-OE1	6.66	1.32	1.25
1	B	21	GLU	CD-OE1	6.60	1.32	1.25
1	A	149	GLU	CD-OE2	6.57	1.32	1.25
1	B	115	GLU	CD-OE2	6.46	1.32	1.25
1	A	333	GLU	CD-OE2	6.42	1.32	1.25
1	D	161	GLU	CD-OE1	6.40	1.32	1.25
1	A	238	GLU	CD-OE1	6.38	1.32	1.25
1	C	149	GLU	CD-OE2	6.37	1.32	1.25
1	C	333	GLU	CD-OE1	6.36	1.32	1.25
1	C	207	GLU	CD-OE1	6.23	1.32	1.25
1	A	140	GLU	CD-OE1	6.22	1.32	1.25
1	B	333	GLU	CD-OE1	6.22	1.32	1.25
1	B	35	GLU	CD-OE1	6.21	1.32	1.25
1	B	105	GLU	CD-OE1	6.18	1.32	1.25
1	A	115	GLU	CD-OE2	6.14	1.32	1.25
1	C	140	GLU	CD-OE1	6.13	1.32	1.25
1	D	145	GLU	CD-OE1	6.13	1.32	1.25
1	D	149	GLU	CD-OE2	6.13	1.32	1.25
1	A	145	GLU	CD-OE2	6.12	1.32	1.25
1	C	105	GLU	CD-OE1	6.12	1.32	1.25
1	C	61	GLU	CD-OE2	6.10	1.32	1.25
1	C	102	GLU	CD-OE1	6.07	1.32	1.25
1	C	145	GLU	CD-OE1	6.04	1.32	1.25
1	D	51	GLU	CD-OE2	6.01	1.32	1.25
1	D	333	GLU	CD-OE1	5.91	1.32	1.25
1	D	115	GLU	CD-OE2	5.89	1.32	1.25
1	C	208	GLU	CD-OE2	5.84	1.32	1.25
1	A	153	GLU	CD-OE1	5.80	1.32	1.25
1	A	102	GLU	CD-OE1	5.78	1.32	1.25
1	C	115	GLU	CD-OE1	5.74	1.31	1.25
1	A	55	GLU	CD-OE2	5.72	1.31	1.25
1	B	226	GLU	CD-OE1	5.70	1.31	1.25
1	A	226	GLU	CD-OE1	5.68	1.31	1.25
1	D	308	GLU	CD-OE1	5.62	1.31	1.25
1	C	51	GLU	CD-OE2	5.61	1.31	1.25
1	B	145	GLU	CD-OE1	5.59	1.31	1.25
1	A	161	GLU	CD-OE1	5.57	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	GLU	CD-OE2	5.56	1.31	1.25
1	B	140	GLU	CD-OE1	5.48	1.31	1.25
1	A	308	GLU	CD-OE1	5.44	1.31	1.25
1	C	21	GLU	CD-OE1	5.42	1.31	1.25
1	D	105	GLU	CD-OE1	5.42	1.31	1.25
1	A	260	GLU	CD-OE1	5.39	1.31	1.25
1	C	342	GLU	CD-OE2	5.34	1.31	1.25
1	C	308	GLU	CD-OE1	5.34	1.31	1.25
1	D	55	GLU	CD-OE2	5.33	1.31	1.25
1	C	138	GLU	CD-OE2	5.32	1.31	1.25
1	D	226	GLU	CD-OE1	5.32	1.31	1.25
1	A	138	GLU	CD-OE1	5.31	1.31	1.25
1	A	216	GLU	CD-OE1	5.29	1.31	1.25
1	B	49	GLU	CD-OE1	5.24	1.31	1.25
1	D	207	GLU	CD-OE1	5.19	1.31	1.25
1	A	207	GLU	CD-OE1	5.17	1.31	1.25
1	D	35	GLU	CD-OE1	5.13	1.31	1.25
1	D	238	GLU	CD-OE1	5.11	1.31	1.25
1	B	308	GLU	CD-OE1	5.08	1.31	1.25
1	A	21	GLU	CD-OE2	-5.07	1.20	1.25
1	B	51	GLU	CD-OE2	5.06	1.31	1.25
1	D	49	GLU	CD-OE1	5.06	1.31	1.25
1	A	105	GLU	CD-OE1	5.03	1.31	1.25

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	TYR	CG-CD1-CE1	10.92	130.04	121.30
1	A	324	ASP	CA-C-N	-10.04	95.12	117.20
1	D	72	ASP	CB-CG-OD1	-9.82	109.46	118.30
1	C	327	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	324	ASP	CB-CG-OD1	-8.42	110.72	118.30
1	A	293	ASP	CB-CG-OD1	-8.42	110.72	118.30
1	D	103	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	147	TYR	CB-CG-CD2	8.09	125.85	121.00
1	A	17	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	D	80	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	D	171	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	C	17	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	C	72	ASP	CB-CG-OD2	7.83	125.35	118.30
1	C	192	SER	N-CA-CB	7.75	122.12	110.50
1	B	242	ARG	NE-CZ-NH1	7.69	124.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	264	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	C	171	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	C	60	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	112	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	80	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	C	306	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	D	72	ASP	CB-CG-OD2	7.38	124.94	118.30
1	D	186	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	14	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	D	190	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	268	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	186	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	C	121	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	14	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	D	223	MET	CG-SD-CE	-7.09	88.86	100.20
1	D	80	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	D	186	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	B	306	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	D	111	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	D	171	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	135	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	306	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	C	111	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	D	88	ASP	CB-CG-OD1	-6.67	112.29	118.30
1	D	289	ASP	CB-CG-OD1	-6.67	112.29	118.30
1	C	114	GLY	O-C-N	-6.67	112.03	122.70
1	B	111	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	D	306	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	324	ASP	O-C-N	6.54	133.16	122.70
1	D	17	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	65	HIS	ND1-CG-CD2	6.51	117.91	108.80
1	C	80	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	111	ASP	CB-CG-OD1	6.44	124.10	118.30
1	B	324	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	C	293	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	D	322	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	310	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	B	135	ARG	N-CA-CB	6.30	121.95	110.60
1	B	190	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	33	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	212	ALA	N-CA-CB	-6.27	101.32	110.10
1	A	88	ASP	CB-CG-OD2	6.24	123.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	72	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	A	111	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	C	205	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	289	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	B	171	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	306	ASP	CB-CG-OD1	6.06	123.75	118.30
1	C	110	PHE	CG-CD2-CE2	6.01	127.41	120.80
1	B	310	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	310	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	310	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	289	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	B	293	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	327	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	306	ASP	CB-CG-OD1	5.94	123.64	118.30
1	C	322	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	C	112	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	C	113	LEU	CB-CA-C	5.90	121.40	110.20
1	D	327	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	33	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	D	322	ASP	CB-CG-OD1	-5.85	113.03	118.30
1	B	324	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	268	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	A	289	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	88	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	C	310	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	63	ALA	N-CA-CB	5.68	118.06	110.10
1	A	279	PRO	N-CA-CB	5.67	110.11	103.30
1	B	293	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	D	135	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	186	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	293	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	72	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	A	135	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	310	ARG	N-CA-CB	5.61	120.70	110.60
1	B	186	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	C	171	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	260	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	A	293	ASP	CB-CG-OD2	5.54	123.28	118.30
1	D	289	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	79	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	147	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
1	B	171	ASP	CB-CG-OD2	-5.49	113.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	SER	N-CA-CB	5.49	118.73	110.50
1	A	80	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	186	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	B	111	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	111	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	289	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	242	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	60	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	103	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	103	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	194	ALA	N-CA-CB	5.31	117.53	110.10
1	D	293	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	251	GLN	N-CA-CB	5.29	120.13	110.60
1	B	72	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	313	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	111	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	72	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	14	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	C	264	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	88	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	289	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	C	260	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	A	147	TYR	CD1-CG-CD2	-5.08	112.31	117.90
1	C	260	GLU	OE1-CD-OE2	5.00	129.30	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	ASP	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	2751	0	2732	158	0
1	B	2784	0	2759	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2747	0	2729	159	0
1	D	2747	0	2729	131	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	107	0	0	4	1
4	B	121	0	0	5	0
4	C	136	0	0	4	0
4	D	127	0	0	5	1
All	All	11632	0	10997	547	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (547) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:PRO:HB2	1:D:235:LEU:HD23	1.46	0.96
1:B:119:VAL:HG22	1:B:152:VAL:HG13	1.47	0.94
1:C:8:GLY:HA3	1:C:49:GLU:HG2	1.54	0.90
1:A:42:GLN:NE2	1:A:42:GLN:H	1.73	0.87
1:A:42:GLN:H	1:A:42:GLN:HE21	1.26	0.83
1:A:81:LEU:HD23	1:A:122:ARG:HH21	1.43	0.82
1:A:355:GLY:HA3	1:C:133:ARG:HH11	1.44	0.82
1:C:99:LEU:HD11	1:C:148:GLY:HA2	1.62	0.80
1:C:144:ALA:HA	1:C:147:TYR:HE1	1.47	0.79
1:A:142:LEU:CD1	1:A:143:PRO:HD2	2.13	0.79
1:A:40:PRO:HA	1:A:42:GLN:HE22	1.47	0.78
1:A:119:VAL:CG2	1:A:132:TRP:HB2	2.14	0.78
1:A:81:LEU:HD12	1:A:97:TRP:HZ3	1.48	0.78
1:A:99:LEU:HD21	1:A:148:GLY:HA2	1.66	0.77
1:D:185:GLN:HE21	1:D:190:ARG:HD2	1.49	0.77
1:A:168:ARG:HG3	1:A:174:THR:HG22	1.65	0.77
1:D:49:GLU:HG3	1:D:50:ILE:HG23	1.67	0.76
1:B:340:PRO:HB2	1:B:342:GLU:OE2	1.85	0.76
1:A:144:ALA:HA	1:A:147:TYR:CE2	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:HG22	1:B:47:THR:CG2	2.15	0.76
1:A:81:LEU:HD12	1:A:97:TRP:CZ3	2.21	0.76
1:A:142:LEU:HD12	1:A:143:PRO:HD2	1.68	0.75
1:C:99:LEU:HD12	1:C:100:LEU:N	2.02	0.75
1:C:96:PRO:HG2	1:C:154:GLN:OE1	1.86	0.75
1:D:137:ASN:ND2	1:D:137:ASN:H	1.83	0.75
1:D:79:ASP:HB3	1:D:82:THR:OG1	1.87	0.75
1:D:116:LEU:HG	1:D:117:ALA:N	2.01	0.74
1:B:86:LEU:HD11	1:B:90:LEU:HD22	1.69	0.74
1:A:65:HIS:CE1	1:A:67:ALA:HB3	2.23	0.74
1:C:144:ALA:HA	1:C:147:TYR:CE1	2.22	0.73
1:A:144:ALA:HA	1:A:147:TYR:CD2	2.22	0.73
1:A:309:VAL:HG22	1:A:315:VAL:HG11	1.70	0.73
1:D:137:ASN:H	1:D:137:ASN:HD22	1.34	0.73
1:B:2:LYS:HG2	1:B:25:ILE:HG12	1.71	0.73
1:D:319:ASN:C	1:D:320:LEU:HD12	2.08	0.73
1:B:102:GLU:O	1:B:105:GLU:HB2	1.89	0.73
1:B:278:ASN:HB3	1:B:279:PRO:HD2	1.70	0.72
1:D:118:ILE:HD13	1:D:155:GLY:HA2	1.71	0.72
1:A:355:GLY:HA3	1:C:133:ARG:NH1	2.05	0.72
1:C:115:GLU:O	1:C:135:ARG:HG2	1.89	0.72
1:A:157:ASN:HB3	1:C:232:GLN:HA	1.71	0.71
1:A:96:PRO:HG2	1:A:154:GLN:OE1	1.91	0.71
1:C:209:MET:O	1:C:212:ALA:HB3	1.91	0.71
1:A:142:LEU:HG	1:A:143:PRO:HD2	1.73	0.70
1:D:143:PRO:HB2	1:D:145:GLU:HG3	1.74	0.70
1:D:3:GLN:HB3	1:D:44:SER:HB3	1.73	0.70
1:C:81:LEU:HD22	1:C:122:ARG:HH21	1.57	0.70
1:A:119:VAL:HG22	1:A:132:TRP:O	1.93	0.69
1:A:36:PRO:HA	1:A:58:LEU:HD13	1.75	0.69
1:B:230:THR:HB	1:B:231:PRO:HD2	1.74	0.69
1:C:340:PRO:HG2	1:C:343:TYR:CE1	2.28	0.69
1:A:142:LEU:CG	1:A:143:PRO:HD2	2.23	0.69
1:D:81:LEU:O	1:D:85:GLN:HG3	1.93	0.69
1:C:139:THR:HG22	1:C:140:GLU:N	2.08	0.68
1:D:102:GLU:O	1:D:105:GLU:HB2	1.93	0.68
1:D:58:LEU:HD12	1:D:62:LEU:HD13	1.76	0.68
1:D:52:ARG:NH2	1:D:123:THR:HG23	2.08	0.68
1:D:93:PRO:CB	1:D:235:LEU:HD23	2.24	0.68
1:B:118:ILE:CD1	1:B:155:GLY:HA2	2.23	0.67
1:B:190:ARG:NH2	4:B:2464:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:VAL:HG11	1:C:39:VAL:HG11	1.75	0.67
1:A:108:ALA:HB1	1:A:112:ARG:NH1	2.09	0.67
1:C:182:ASN:HD21	1:C:246:SER:HB2	1.57	0.67
1:C:278:ASN:HB3	1:C:279:PRO:HD2	1.76	0.67
1:D:291:ASN:HB3	1:D:294:TRP:CE2	2.30	0.66
1:D:289:ASP:OD1	1:D:309:VAL:HG21	1.95	0.66
1:D:106:TRP:O	1:D:109:VAL:HB	1.96	0.66
1:A:230:THR:HB	1:A:231:PRO:HD2	1.78	0.66
1:C:81:LEU:O	1:C:85:GLN:HG3	1.95	0.66
1:D:56:THR:O	1:D:60:ARG:HG3	1.96	0.65
1:B:86:LEU:CD1	1:B:90:LEU:HD22	2.25	0.65
1:B:168:ARG:HG3	1:B:174:THR:HG22	1.77	0.65
1:D:84:LYS:NZ	1:D:153:GLU:OE2	2.30	0.65
1:A:191:THR:HG22	1:A:349:TRP:CZ3	2.32	0.65
1:B:242:ARG:HG3	1:B:243:VAL:O	1.96	0.65
1:A:337:PRO:HA	1:C:348:ILE:CD1	2.27	0.65
1:C:252:ASN:HB2	4:C:2310:HOH:O	1.96	0.65
1:C:51:GLU:N	1:C:51:GLU:OE1	2.29	0.65
1:D:3:GLN:CB	1:D:44:SER:HB3	2.27	0.65
1:D:135:ARG:N	1:D:138:GLU:OE1	2.30	0.64
1:B:138:GLU:O	1:B:141:GLN:HB2	1.97	0.64
1:C:182:ASN:HB3	1:C:189:LEU:CD1	2.28	0.64
1:B:135:ARG:N	1:B:138:GLU:OE1	2.30	0.64
1:D:84:LYS:HB3	1:D:97:TRP:CE2	2.32	0.64
1:C:308:GLU:O	1:C:313:ARG:NH1	2.31	0.63
1:D:209:MET:CE	1:D:236:ILE:HG13	2.28	0.63
1:C:65:HIS:HE1	1:C:67:ALA:HB3	1.64	0.63
1:A:227:CYS:HB3	1:A:234:LEU:HD23	1.79	0.63
1:D:106:TRP:NE1	1:D:139:THR:HG23	2.13	0.63
1:C:99:LEU:CD1	1:C:148:GLY:HA2	2.27	0.63
1:B:333:GLU:HA	1:B:336:ILE:HD12	1.80	0.63
1:D:191:THR:HG22	1:D:349:TRP:HZ3	1.62	0.63
1:B:34:ALA:HB3	1:B:58:LEU:HD22	1.80	0.62
1:B:6:VAL:HG22	1:B:47:THR:HG23	1.81	0.62
1:A:93:PRO:HG2	1:A:209:MET:HE3	1.81	0.62
1:A:191:THR:HG22	1:A:349:TRP:HZ3	1.63	0.62
1:B:216:GLU:O	1:B:216:GLU:HG3	1.99	0.62
1:C:98:GLN:HG2	1:C:152:VAL:HG23	1.82	0.62
1:C:118:ILE:CD1	1:C:155:GLY:HA2	2.29	0.62
1:B:119:VAL:HG22	1:B:152:VAL:CG1	2.25	0.62
1:B:205:ARG:O	1:B:209:MET:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:OE1	1:A:38:ALA:HB2	2.00	0.62
1:A:291:ASN:HB3	1:A:294:TRP:CE2	2.35	0.62
1:C:56:THR:O	1:C:60:ARG:HB2	2.00	0.62
1:A:3:GLN:HB3	1:A:44:SER:HB3	1.82	0.62
1:D:185:GLN:HB2	1:D:190:ARG:HD2	1.80	0.62
1:B:72:ASP:O	1:B:75:PRO:HD2	2.00	0.62
1:C:80:ARG:HH12	1:C:238:GLU:HG3	1.65	0.61
1:D:21:GLU:HB3	1:D:22:PRO:HD3	1.82	0.61
1:A:119:VAL:O	1:A:131:GLN:HA	2.00	0.61
1:C:8:GLY:HA3	1:C:49:GLU:CG	2.30	0.61
1:B:264:ARG:O	1:B:269:LEU:N	2.30	0.61
1:B:118:ILE:HD13	1:B:155:GLY:HA2	1.83	0.60
1:C:138:GLU:HB3	1:C:141:GLN:OE1	2.02	0.59
1:B:90:LEU:HB3	1:B:92:LEU:HG	1.83	0.59
1:B:182:ASN:ND2	1:B:192:SER:HB3	2.17	0.59
1:C:340:PRO:HG2	1:C:343:TYR:HE1	1.66	0.59
1:D:340:PRO:HB2	1:D:342:GLU:OE2	2.02	0.59
1:C:290:VAL:HG22	1:C:304:TRP:CE3	2.37	0.59
1:D:282:MET:HG2	1:D:283:ILE:N	2.18	0.59
1:A:158:PHE:CE1	1:A:161:GLU:HG3	2.37	0.59
1:B:4:VAL:O	1:B:27:VAL:HA	2.03	0.59
1:B:193:VAL:HG22	1:B:281:VAL:HG22	1.84	0.59
1:D:302:LEU:HD12	1:D:303:HIS:N	2.18	0.59
1:C:81:LEU:HD22	1:C:122:ARG:NH2	2.17	0.59
1:A:70:ASN:ND2	1:A:220:VAL:O	2.30	0.58
1:B:115:GLU:H	1:B:115:GLU:CD	2.06	0.58
1:B:77:ILE:HD13	1:B:77:ILE:N	2.19	0.58
1:A:81:LEU:CD2	1:A:122:ARG:HH21	2.16	0.58
1:B:285:LEU:HD11	1:B:318:LEU:HD21	1.84	0.58
1:C:322:ASP:OD2	1:C:327:ARG:HD2	2.04	0.57
1:D:322:ASP:CG	1:D:327:ARG:HH21	2.06	0.57
1:A:102:GLU:HB3	1:A:104:SER:OG	2.03	0.57
1:B:76:ILE:HG22	1:B:77:ILE:HD13	1.86	0.57
1:C:96:PRO:O	1:C:153:GLU:HA	2.03	0.57
1:A:99:LEU:HG	1:A:100:LEU:N	2.19	0.57
1:A:106:TRP:N	1:A:107:PRO:HD2	2.20	0.57
1:A:108:ALA:O	1:A:112:ARG:NH1	2.38	0.57
1:B:50:ILE:HD12	1:B:52:ARG:O	2.05	0.57
1:B:21:GLU:HB3	1:B:22:PRO:HD3	1.87	0.57
1:C:92:LEU:HB3	1:C:236:ILE:HD12	1.87	0.57
1:D:209:MET:HE3	1:D:236:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:CD1	1:A:97:TRP:HZ3	2.18	0.57
1:B:287:GLY:HA2	1:B:310:ARG:O	2.04	0.57
1:D:278:ASN:HB3	1:D:279:PRO:HD2	1.87	0.57
1:A:55:GLU:O	1:A:55:GLU:HG2	2.03	0.56
1:C:213:ILE:HG21	1:C:239:LEU:HD21	1.86	0.56
1:D:6:VAL:HG22	1:D:47:THR:CG2	2.35	0.56
1:A:97:TRP:HA	1:A:152:VAL:O	2.06	0.56
1:B:309:VAL:HG22	1:B:315:VAL:HG11	1.87	0.56
1:D:56:THR:OG1	1:D:59:THR:HG23	2.06	0.56
1:D:185:GLN:NE2	1:D:190:ARG:HD2	2.19	0.56
1:D:292:TYR:O	1:D:295:LEU:HB2	2.05	0.56
1:A:56:THR:O	1:A:60:ARG:HB2	2.06	0.56
1:B:129:ARG:HG3	1:B:130:GLY:N	2.20	0.56
1:D:302:LEU:HD12	1:D:303:HIS:H	1.69	0.56
1:B:190:ARG:NE	1:B:286:ILE:HD13	2.20	0.56
1:C:292:TYR:HD1	1:C:295:LEU:HD22	1.71	0.56
1:A:45:VAL:O	1:A:46:ILE:HD13	2.06	0.56
1:D:118:ILE:CD1	1:D:155:GLY:HA2	2.36	0.55
1:A:319:ASN:C	1:A:320:LEU:HD12	2.27	0.55
1:A:92:LEU:HD22	1:A:209:MET:HG2	1.88	0.55
1:C:55:GLU:HG3	1:C:60:ARG:HG3	1.88	0.55
1:D:6:VAL:HG22	1:D:47:THR:HG22	1.88	0.55
1:A:243:VAL:HG22	4:A:2006:HOH:O	2.06	0.55
1:C:99:LEU:HD11	1:C:148:GLY:CA	2.34	0.55
1:C:106:TRP:NE1	1:C:139:THR:HG23	2.21	0.55
1:C:110:PHE:HD2	1:C:114:GLY:O	1.89	0.55
1:D:4:VAL:O	1:D:27:VAL:HA	2.06	0.55
1:D:320:LEU:HD12	1:D:320:LEU:N	2.21	0.55
1:B:282:MET:HG2	1:B:283:ILE:N	2.22	0.55
1:A:108:ALA:O	1:A:111:ASP:HB3	2.07	0.55
1:A:89:LYS:HG2	1:A:90:LEU:CD1	2.36	0.54
1:D:191:THR:HG22	1:D:349:TRP:CZ3	2.41	0.54
1:D:103:ARG:NH2	4:D:2425:HOH:O	2.29	0.54
1:A:65:HIS:HE1	1:A:67:ALA:HB3	1.70	0.54
1:C:68:PHE:CD2	1:C:71:ARG:HG3	2.43	0.54
1:C:286:ILE:HA	1:C:313:ARG:O	2.08	0.54
1:D:184:HIS:HA	1:D:188:ILE:O	2.07	0.54
1:A:184:HIS:HA	1:A:188:ILE:O	2.08	0.54
1:A:201:GLN:HA	1:A:201:GLN:OE1	2.07	0.54
1:B:81:LEU:HD23	1:B:122:ARG:NH2	2.23	0.54
1:B:168:ARG:HG3	1:B:174:THR:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:HA	1:A:147:TYR:HE2	1.70	0.54
1:B:21:GLU:HB3	1:B:22:PRO:CD	2.37	0.53
1:C:278:ASN:HB3	1:C:279:PRO:CD	2.39	0.53
1:A:74:PHE:HB2	1:A:75:PRO:HD3	1.89	0.53
1:C:11:GLN:O	1:C:15:MET:HE2	2.08	0.53
1:A:332:LEU:O	1:A:335:LEU:HB2	2.08	0.53
1:C:219:TYR:CE2	1:C:223:MET:HB2	2.44	0.53
1:C:238:GLU:HG2	4:C:2170:HOH:O	2.07	0.53
1:C:292:TYR:O	1:C:295:LEU:HB2	2.08	0.53
1:D:185:GLN:O	1:D:186:ASP:HB2	2.09	0.53
1:C:291:ASN:HB3	1:C:294:TRP:CE2	2.44	0.53
1:A:138:GLU:HG2	1:A:141:GLN:OE1	2.09	0.52
1:A:298:PRO:HD2	4:A:2027:HOH:O	2.10	0.52
1:C:134:LEU:HG	1:C:138:GLU:O	2.09	0.52
1:C:116:LEU:HD23	1:C:117:ALA:N	2.23	0.52
1:D:137:ASN:ND2	1:D:137:ASN:N	2.56	0.52
1:A:226:GLU:HB3	4:A:2155:HOH:O	2.09	0.52
1:C:11:GLN:HG2	1:C:12:LEU:N	2.25	0.52
1:D:99:LEU:HA	1:D:151:ILE:HG22	1.91	0.52
1:C:288:SER:HG	1:C:343:TYR:HH	1.57	0.52
1:B:64:ARG:NH1	4:B:2088:HOH:O	2.42	0.52
1:C:96:PRO:HD2	1:C:154:GLN:HB3	1.92	0.51
1:C:108:ALA:O	1:C:111:ASP:N	2.30	0.51
1:B:184:HIS:HA	1:B:188:ILE:O	2.10	0.51
1:A:182:ASN:HB3	1:A:189:LEU:CD1	2.39	0.51
1:C:230:THR:HB	1:C:231:PRO:HD2	1.92	0.51
1:D:245:ASN:HA	1:D:248:HIS:CE1	2.45	0.51
1:A:336:ILE:N	1:A:337:PRO:HD2	2.26	0.51
1:C:3:GLN:HG2	1:C:26:ALA:HB3	1.92	0.51
1:D:182:ASN:HB3	1:D:189:LEU:CD1	2.40	0.51
1:B:128:GLY:N	3:B:1200:ADP:O1B	2.39	0.51
1:C:74:PHE:N	1:C:75:PRO:HD2	2.26	0.51
1:B:190:ARG:CZ	1:B:286:ILE:HD13	2.41	0.51
1:C:336:ILE:HB	1:C:337:PRO:HD3	1.93	0.51
1:A:144:ALA:O	1:A:147:TYR:HD2	1.93	0.51
1:A:40:PRO:CA	1:A:42:GLN:HE22	2.22	0.50
1:A:284:ASN:HB3	1:A:286:ILE:HD11	1.92	0.50
1:B:137:ASN:OD1	1:B:137:ASN:N	2.44	0.50
1:C:109:VAL:HG13	1:C:113:LEU:HD12	1.93	0.50
1:D:58:LEU:CD1	1:D:62:LEU:HD13	2.40	0.50
1:A:337:PRO:HA	1:C:348:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:TRP:CE3	1:C:142:LEU:HD11	2.46	0.50
1:C:139:THR:O	1:C:141:GLN:N	2.44	0.50
1:C:286:ILE:HG22	1:C:286:ILE:O	2.10	0.50
1:D:76:ILE:HG22	1:D:77:ILE:HD13	1.93	0.50
1:B:230:THR:CB	1:B:231:PRO:HD2	2.37	0.50
1:B:336:ILE:N	1:B:337:PRO:HD2	2.27	0.49
1:C:90:LEU:HD11	1:C:216:GLU:HG2	1.93	0.49
1:C:102:GLU:HB3	1:C:104:SER:OG	2.13	0.49
1:B:14:ARG:O	1:B:18:GLN:HG3	2.12	0.49
1:B:126:TYR:OH	1:B:129:ARG:NH1	2.45	0.49
1:D:106:TRP:N	1:D:107:PRO:HD2	2.28	0.49
1:C:160:GLY:O	1:C:229:VAL:HB	2.12	0.49
1:A:110:PHE:CE1	1:A:136:ALA:N	2.81	0.49
1:C:290:VAL:HG22	1:C:304:TRP:CZ3	2.47	0.49
1:A:45:VAL:C	1:A:46:ILE:HD13	2.33	0.49
1:A:76:ILE:O	1:A:82:THR:OG1	2.30	0.49
1:C:106:TRP:O	1:C:110:PHE:HD1	1.95	0.49
1:A:191:THR:HG21	1:A:350:ALA:HB2	1.94	0.49
1:C:182:ASN:HB3	1:C:189:LEU:HD11	1.95	0.49
1:A:119:VAL:HG23	1:A:132:TRP:HB2	1.92	0.49
1:D:106:TRP:HA	1:D:106:TRP:CE3	2.47	0.49
1:B:80:ARG:HH12	1:B:238:GLU:CG	2.26	0.49
1:D:84:LYS:HZ2	1:D:153:GLU:CD	2.14	0.49
1:D:209:MET:HE3	1:D:236:ILE:CD1	2.43	0.49
1:B:324:ASP:OD1	1:B:326:SER:OG	2.30	0.48
1:C:77:ILE:CD1	1:C:239:LEU:HD23	2.42	0.48
1:D:245:ASN:HB2	4:D:2411:HOH:O	2.13	0.48
1:A:245:ASN:OD1	1:A:314:LYS:NZ	2.39	0.48
1:B:118:ILE:HG13	1:B:133:ARG:HG2	1.95	0.48
1:B:336:ILE:HB	1:B:337:PRO:HD3	1.94	0.48
1:A:35:GLU:CD	1:A:35:GLU:H	2.14	0.48
1:B:105:GLU:HG2	4:B:2459:HOH:O	2.12	0.48
1:C:295:LEU:HG	1:D:264:ARG:NH2	2.28	0.48
1:D:199:ASN:OD1	1:D:202:GLN:HB2	2.13	0.48
1:A:89:LYS:HG2	1:A:90:LEU:HD13	1.95	0.48
1:A:176:PHE:HE1	1:A:210:LEU:HD23	1.78	0.48
1:C:14:ARG:NH2	1:C:304:TRP:O	2.46	0.48
1:C:99:LEU:HD12	1:C:100:LEU:C	2.34	0.48
1:C:100:LEU:HD12	1:C:100:LEU:HA	1.69	0.48
1:C:119:VAL:O	1:C:131:GLN:HB2	2.13	0.48
1:D:322:ASP:OD2	1:D:324:ASP:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:O	1:A:141:GLN:HB2	2.12	0.48
1:A:138:GLU:O	1:A:141:GLN:N	2.30	0.48
1:B:285:LEU:HD21	1:B:318:LEU:HG	1.94	0.48
1:C:194:ALA:O	1:C:279:PRO:HA	2.14	0.48
1:C:65:HIS:CE1	1:C:67:ALA:HB3	2.45	0.48
1:C:121:ARG:NH2	1:C:132:TRP:CH2	2.82	0.48
1:A:142:LEU:HG	1:A:143:PRO:CD	2.43	0.47
1:B:179:LEU:HD11	1:B:203:GLN:HA	1.95	0.47
1:B:292:TYR:O	1:B:295:LEU:HB2	2.14	0.47
1:D:116:LEU:HG	1:D:117:ALA:H	1.77	0.47
1:D:288:SER:OG	1:D:343:TYR:OH	2.29	0.47
1:C:325:THR:O	1:C:329:THR:HG23	2.14	0.47
1:D:264:ARG:HB3	1:D:271:LEU:HD13	1.96	0.47
1:A:79:ASP:OD1	1:A:81:LEU:HB3	2.15	0.47
1:B:269:LEU:HB3	1:B:270:PRO:HD2	1.96	0.47
1:D:79:ASP:OD1	1:D:81:LEU:HB3	2.14	0.47
1:C:207:GLU:O	1:C:211:SER:OG	2.30	0.47
1:D:95:ALA:CB	1:D:153:GLU:HG2	2.44	0.47
1:B:100:LEU:O	1:B:148:GLY:N	2.39	0.47
1:C:92:LEU:HB3	1:C:236:ILE:CD1	2.45	0.47
1:D:344:ALA:O	1:D:348:ILE:HD12	2.14	0.47
1:C:97:TRP:HA	1:C:152:VAL:O	2.15	0.47
1:C:99:LEU:HB2	1:C:151:ILE:HG22	1.97	0.47
1:C:101:ALA:O	1:C:147:TYR:HD2	1.98	0.47
1:D:322:ASP:OD1	1:D:327:ARG:NH2	2.47	0.47
1:A:80:ARG:HH12	1:A:238:GLU:HG3	1.79	0.47
1:A:105:GLU:C	1:A:107:PRO:HD2	2.35	0.47
1:B:103:ARG:C	1:B:105:GLU:H	2.17	0.47
1:B:328:LEU:HA	1:B:328:LEU:HD12	1.51	0.47
1:C:119:VAL:HG12	1:C:132:TRP:CE3	2.49	0.47
1:C:289:ASP:HB2	4:C:2292:HOH:O	2.14	0.47
1:D:95:ALA:HB3	1:D:153:GLU:HG2	1.96	0.47
1:B:291:ASN:ND2	1:B:293:ASP:HB2	2.30	0.47
1:B:298:PRO:HD2	4:B:2109:HOH:O	2.14	0.47
1:D:39:VAL:C	1:D:41:PHE:H	2.17	0.47
1:C:109:VAL:O	1:C:113:LEU:N	2.48	0.46
1:D:137:ASN:ND2	4:D:2424:HOH:O	2.48	0.46
1:B:285:LEU:O	1:B:315:VAL:HG22	2.16	0.46
1:D:168:ARG:HG3	1:D:174:THR:HG22	1.96	0.46
1:D:335:LEU:O	1:D:338:LEU:HB2	2.14	0.46
1:A:98:GLN:HE21	1:A:98:GLN:HB2	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:O	1:A:207:GLU:HG3	2.16	0.46
1:C:94:THR:C	1:C:235:LEU:HD23	2.36	0.46
1:A:202:GLN:HG2	1:A:234:LEU:HD11	1.96	0.46
1:A:355:GLY:CA	1:C:133:ARG:HD3	2.44	0.46
1:C:336:ILE:CB	1:C:337:PRO:HD3	2.46	0.46
1:D:12:LEU:HB2	1:D:49:GLU:OE1	2.15	0.46
1:B:317:HIS:C	1:B:318:LEU:HD23	2.36	0.46
1:C:145:GLU:C	1:C:147:TYR:H	2.17	0.46
1:D:90:LEU:HD23	1:D:92:LEU:HD11	1.96	0.46
1:A:324:ASP:O	1:A:328:LEU:HB2	2.16	0.46
1:C:73:VAL:C	1:C:75:PRO:HD2	2.36	0.46
1:C:267:THR:O	1:C:268:ASP:HB2	2.16	0.46
1:D:79:ASP:O	1:D:82:THR:OG1	2.30	0.46
1:D:194:ALA:O	1:D:279:PRO:HA	2.15	0.46
1:C:30:VAL:CG1	1:C:39:VAL:HG11	2.45	0.46
1:C:121:ARG:NH2	1:C:132:TRP:CZ2	2.84	0.46
1:D:99:LEU:HB3	4:D:2183:HOH:O	2.15	0.46
1:A:84:LYS:HE3	1:A:97:TRP:CD1	2.50	0.46
1:A:119:VAL:HG21	1:A:132:TRP:HB2	1.95	0.46
1:A:264:ARG:HA	1:A:269:LEU:HB2	1.96	0.46
1:C:21:GLU:HG2	1:D:18:GLN:NE2	2.31	0.46
1:D:309:VAL:HG23	4:D:2384:HOH:O	2.14	0.46
1:A:142:LEU:HD12	1:A:143:PRO:CD	2.42	0.46
1:B:79:ASP:HB3	1:B:82:THR:OG1	2.16	0.46
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.44	0.46
1:B:285:LEU:HD11	1:B:318:LEU:CD2	2.46	0.46
1:C:100:LEU:HD21	1:C:106:TRP:CZ2	2.51	0.46
1:A:256:ILE:HG21	1:A:261:LEU:HD13	1.97	0.45
1:C:241:PRO:O	1:C:242:ARG:HB3	2.15	0.45
1:C:264:ARG:HA	1:C:269:LEU:HB2	1.98	0.45
1:C:328:LEU:HA	1:C:328:LEU:HD12	1.74	0.45
1:D:68:PHE:HD1	1:D:69:VAL:N	2.14	0.45
1:D:158:PHE:HB3	1:D:228:PHE:HB3	1.97	0.45
1:D:263:LEU:O	1:D:267:THR:HG23	2.16	0.45
1:A:139:THR:HB	4:A:2011:HOH:O	2.16	0.45
1:B:9:ASN:HD22	1:B:9:ASN:HA	1.45	0.45
1:C:131:GLN:O	1:C:131:GLN:HG3	2.15	0.45
1:C:145:GLU:O	1:C:147:TYR:N	2.41	0.45
1:C:249:TRP:CH2	1:C:250:THR:HG22	2.51	0.45
1:D:245:ASN:OD1	1:D:314:LYS:HE2	2.15	0.45
1:A:243:VAL:CG1	1:A:258:GLN:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:TRP:CE3	1:C:142:LEU:CD1	3.00	0.45
1:D:106:TRP:N	1:D:107:PRO:CD	2.80	0.45
1:A:21:GLU:CB	1:A:22:PRO:HD3	2.47	0.45
1:A:355:GLY:C	1:C:133:ARG:HD3	2.36	0.45
1:D:32:LEU:HD13	1:D:54:PRO:HD2	1.97	0.45
1:D:119:VAL:O	1:D:131:GLN:HB2	2.16	0.45
1:A:60:ARG:O	1:A:63:ALA:HB3	2.15	0.45
1:B:245:ASN:HA	1:B:248:HIS:CE1	2.52	0.45
1:C:132:TRP:CD2	1:C:142:LEU:CD1	3.00	0.45
1:C:182:ASN:ND2	1:C:246:SER:HB2	2.28	0.45
1:A:288:SER:HG	1:A:343:TYR:HH	1.62	0.45
1:B:321:THR:O	1:B:322:ASP:HB2	2.17	0.45
1:C:106:TRP:NE1	1:C:139:THR:CG2	2.80	0.45
1:D:132:TRP:HB3	1:D:134:LEU:HD13	1.99	0.45
1:D:240:ALA:HA	1:D:241:PRO:HD3	1.73	0.45
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.71	0.45
1:A:74:PHE:N	1:A:75:PRO:CD	2.80	0.45
1:A:108:ALA:CA	1:A:112:ARG:NH1	2.80	0.45
1:A:355:GLY:HA3	1:C:133:ARG:HD3	1.98	0.45
1:B:264:ARG:HD3	1:B:270:PRO:O	2.17	0.45
1:D:245:ASN:ND2	1:D:248:HIS:CD2	2.85	0.45
1:A:101:ALA:O	1:A:147:TYR:HD1	2.00	0.44
1:A:106:TRP:N	1:A:107:PRO:CD	2.80	0.44
1:A:157:ASN:HB3	1:C:232:GLN:CA	2.44	0.44
1:B:308:GLU:O	1:B:313:ARG:NH1	2.39	0.44
1:C:74:PHE:N	1:C:75:PRO:CD	2.80	0.44
1:D:145:GLU:H	1:D:145:GLU:HG2	1.43	0.44
1:D:336:ILE:HG13	1:D:347:VAL:HG11	1.99	0.44
1:A:68:PHE:O	1:A:71:ARG:HB2	2.17	0.44
1:B:210:LEU:O	1:B:213:ILE:HB	2.17	0.44
1:A:295:LEU:HA	1:A:295:LEU:HD12	1.72	0.44
1:C:32:LEU:H	1:C:32:LEU:HG	1.49	0.44
1:D:74:PHE:N	1:D:75:PRO:CD	2.80	0.44
1:D:207:GLU:O	1:D:211:SER:OG	2.35	0.44
1:A:6:VAL:O	1:A:30:VAL:N	2.49	0.44
1:A:342:GLU:H	1:A:342:GLU:HG3	1.24	0.44
1:B:182:ASN:ND2	1:B:192:SER:CB	2.80	0.44
1:C:210:LEU:O	1:C:214:MET:HG3	2.17	0.44
1:D:239:LEU:HD12	1:D:239:LEU:HA	1.60	0.44
1:A:18:GLN:NE2	1:B:21:GLU:OE2	2.35	0.44
1:D:295:LEU:HD12	1:D:295:LEU:HA	1.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:HG3	1:A:60:ARG:HG3	2.00	0.44
1:A:21:GLU:HG2	1:B:18:GLN:NE2	2.32	0.44
1:A:320:LEU:HD12	1:A:320:LEU:N	2.33	0.44
1:A:336:ILE:N	1:A:337:PRO:CD	2.81	0.44
1:C:335:LEU:HA	1:C:335:LEU:HD23	1.82	0.44
1:D:106:TRP:CE2	1:D:139:THR:HG23	2.52	0.44
1:D:223:MET:HE2	1:D:241:PRO:HA	2.00	0.44
1:B:185:GLN:N	1:B:188:ILE:O	2.40	0.44
1:C:139:THR:C	1:C:141:GLN:H	2.21	0.44
1:D:59:THR:O	1:D:63:ALA:N	2.41	0.44
1:D:73:VAL:C	1:D:75:PRO:HD2	2.38	0.44
1:A:61:GLU:OE1	1:A:64:ARG:NH2	2.50	0.44
1:A:81:LEU:HD23	1:A:122:ARG:NH2	2.22	0.44
1:A:84:LYS:HE3	1:A:97:TRP:CG	2.52	0.44
1:A:103:ARG:HG2	1:A:147:TYR:CE1	2.53	0.44
1:A:116:LEU:HD23	1:A:118:ILE:HD12	2.00	0.44
1:C:21:GLU:HG2	1:D:18:GLN:HE21	1.83	0.44
1:C:101:ALA:O	1:C:147:TYR:HB3	2.17	0.44
1:D:105:GLU:C	1:D:107:PRO:HD2	2.38	0.44
1:A:8:GLY:HA3	1:A:49:GLU:CG	2.47	0.43
1:B:291:ASN:HD21	1:B:293:ASP:HB2	1.83	0.43
1:C:319:ASN:HB3	4:C:2310:HOH:O	2.17	0.43
1:D:90:LEU:HB3	1:D:92:LEU:HG	1.98	0.43
1:D:180:THR:CG2	1:D:192:SER:HB3	2.48	0.43
1:A:106:TRP:CD1	1:A:139:THR:CG2	3.02	0.43
1:A:182:ASN:ND2	1:A:192:SER:OG	2.51	0.43
1:B:60:ARG:O	1:B:64:ARG:HD2	2.19	0.43
1:B:329:THR:HA	1:B:332:LEU:HD12	2.00	0.43
1:C:6:VAL:HG22	1:C:47:THR:CG2	2.47	0.43
1:C:119:VAL:HG12	1:C:132:TRP:HE3	1.83	0.43
1:C:168:ARG:HA	1:C:173:SER:O	2.18	0.43
1:D:119:VAL:O	1:D:131:GLN:HA	2.19	0.43
1:D:137:ASN:HD22	1:D:137:ASN:N	2.07	0.43
1:B:106:TRP:N	1:B:107:PRO:CD	2.80	0.43
1:B:182:ASN:HD22	1:B:192:SER:CB	2.32	0.43
1:C:56:THR:OG1	1:C:59:THR:HG23	2.18	0.43
1:C:81:LEU:HD12	1:C:97:TRP:HZ3	1.83	0.43
1:C:324:ASP:OD1	1:C:326:SER:HB2	2.19	0.43
1:A:3:GLN:HG2	1:A:26:ALA:HB3	2.00	0.43
1:A:144:ALA:CA	1:A:147:TYR:HD2	2.32	0.43
1:A:336:ILE:CB	1:A:337:PRO:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:LEU:HA	1:D:58:LEU:HD23	2.00	0.43
1:A:119:VAL:O	1:A:119:VAL:HG23	2.18	0.43
1:C:336:ILE:HG22	1:C:337:PRO:N	2.32	0.43
1:D:74:PHE:N	1:D:75:PRO:HD2	2.34	0.43
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.81	0.43
1:B:2:LYS:HE2	1:B:267:THR:HB	2.00	0.43
1:B:271:LEU:HD12	1:B:271:LEU:HA	1.68	0.43
1:C:2:LYS:HE3	1:C:269:LEU:HD11	2.00	0.43
1:C:106:TRP:CD1	1:C:139:THR:HG21	2.54	0.43
1:B:39:VAL:C	1:B:41:PHE:H	2.22	0.43
1:C:195:PHE:CZ	1:C:354:PHE:CE1	3.07	0.43
1:D:168:ARG:HG3	1:D:174:THR:CG2	2.49	0.43
1:A:108:ALA:CB	1:A:112:ARG:NH1	2.80	0.43
1:A:301:HIS:HB2	1:A:319:ASN:HB2	2.01	0.43
1:C:100:LEU:O	1:C:147:TYR:HA	2.19	0.43
1:D:77:ILE:HD13	1:D:77:ILE:N	2.34	0.43
1:A:81:LEU:CD2	1:A:122:ARG:NH2	2.82	0.43
1:A:83:GLN:O	1:A:86:LEU:HB3	2.19	0.43
1:A:110:PHE:HE1	1:A:135:ARG:HA	1.83	0.43
1:B:196:PRO:HG3	1:B:278:ASN:HA	2.01	0.43
1:C:17:ARG:HA	1:C:27:VAL:HB	2.01	0.43
1:D:39:VAL:HA	1:D:40:PRO:HD3	1.84	0.43
1:A:291:ASN:C	1:A:293:ASP:H	2.22	0.42
1:C:21:GLU:HB3	1:C:22:PRO:HD3	2.01	0.42
1:D:90:LEU:HD12	1:D:90:LEU:HA	1.83	0.42
1:A:90:LEU:CD1	1:A:90:LEU:N	2.82	0.42
1:A:157:ASN:HB3	1:C:232:GLN:CB	2.49	0.42
1:A:288:SER:OG	1:A:343:TYR:OH	2.35	0.42
1:A:336:ILE:HG22	1:A:337:PRO:N	2.33	0.42
1:C:287:GLY:HA2	1:C:310:ARG:O	2.19	0.42
1:C:336:ILE:HD11	1:C:347:VAL:CG1	2.49	0.42
1:D:158:PHE:CD2	1:D:228:PHE:CD1	3.07	0.42
1:B:7:LEU:HB3	1:B:48:ALA:CB	2.49	0.42
1:B:63:ALA:HA	1:B:68:PHE:HD2	1.84	0.42
1:C:21:GLU:CB	1:C:22:PRO:HD3	2.49	0.42
1:D:329:THR:O	1:D:332:LEU:HB2	2.18	0.42
1:A:120:LYS:HA	1:A:130:GLY:O	2.20	0.42
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.68	0.42
1:D:21:GLU:N	1:D:22:PRO:HD2	2.35	0.42
1:A:116:LEU:CD2	1:A:118:ILE:HD12	2.49	0.42
1:A:282:MET:HG2	1:A:283:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HA	1:B:23:LEU:HD12	1.65	0.42
1:B:106:TRP:O	1:B:109:VAL:HB	2.20	0.42
1:C:62:LEU:HA	1:C:62:LEU:HD12	1.73	0.42
1:C:282:MET:HG2	1:C:283:ILE:N	2.32	0.42
1:D:164:LEU:HB2	1:D:179:LEU:HD23	2.00	0.42
1:A:108:ALA:C	1:A:112:ARG:HH11	2.23	0.42
1:B:86:LEU:HD11	1:B:90:LEU:CD2	2.45	0.42
1:C:119:VAL:CG1	1:C:132:TRP:CE3	3.03	0.42
1:A:41:PHE:N	1:A:42:GLN:HE21	2.18	0.42
1:A:185:GLN:HB2	1:A:190:ARG:HG3	2.01	0.42
1:D:182:ASN:ND2	1:D:192:SER:HB3	2.34	0.42
1:A:336:ILE:HG22	1:A:337:PRO:HD3	2.01	0.42
1:A:74:PHE:N	1:A:75:PRO:HD2	2.35	0.42
1:C:32:LEU:HD21	1:C:50:ILE:CD1	2.50	0.42
1:C:119:VAL:CG1	1:C:132:TRP:HE3	2.31	0.42
1:A:144:ALA:HA	1:A:147:TYR:HD2	1.76	0.41
1:A:164:LEU:HD12	1:A:165:VAL:N	2.33	0.41
1:B:291:ASN:HB3	1:B:294:TRP:CE2	2.55	0.41
1:A:205:ARG:HD2	1:A:205:ARG:O	2.20	0.41
1:C:96:PRO:O	1:C:154:GLN:N	2.44	0.41
1:B:28:TRP:CE2	1:B:40:PRO:HG2	2.55	0.41
1:C:118:ILE:HD13	1:C:155:GLY:HA2	2.02	0.41
1:C:320:LEU:HD12	1:C:320:LEU:N	2.35	0.41
1:D:52:ARG:NH2	1:D:123:THR:CG2	2.79	0.41
1:D:106:TRP:HB2	1:D:107:PRO:HD3	2.03	0.41
1:D:335:LEU:HD23	1:D:335:LEU:HA	1.76	0.41
1:A:227:CYS:CB	1:A:234:LEU:HD23	2.46	0.41
1:B:344:ALA:O	1:B:348:ILE:HD12	2.21	0.41
1:C:60:ARG:O	1:C:63:ALA:HB3	2.19	0.41
1:D:4:VAL:HB	1:D:27:VAL:HG22	2.03	0.41
1:D:106:TRP:CD1	1:D:139:THR:HG21	2.55	0.41
1:A:340:PRO:HA	1:A:341:PRO:HD3	1.87	0.41
1:C:46:ILE:HD12	1:C:65:HIS:CE1	2.55	0.41
1:B:241:PRO:O	1:B:242:ARG:HB3	2.19	0.41
1:B:273:GLN:NE2	4:B:2147:HOH:O	2.52	0.41
1:B:278:ASN:HB3	1:B:279:PRO:CD	2.43	0.41
1:D:209:MET:CE	1:D:236:ILE:CD1	2.99	0.41
1:A:144:ALA:CA	1:A:147:TYR:CD2	3.00	0.41
1:B:7:LEU:HB3	1:B:48:ALA:HB2	2.03	0.41
1:C:158:PHE:CD2	1:C:228:PHE:CD1	3.08	0.41
1:C:336:ILE:N	1:C:337:PRO:HD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:O	1:A:30:VAL:HG12	2.20	0.41
1:A:209:MET:HG2	1:A:236:ILE:HD11	2.02	0.41
1:A:243:VAL:HG12	1:A:258:GLN:HG3	2.03	0.41
1:B:63:ALA:HB1	1:B:71:ARG:NH2	2.36	0.41
1:B:79:ASP:OD1	1:B:81:LEU:HB3	2.20	0.41
1:B:151:ILE:HG13	1:B:152:VAL:N	2.34	0.41
1:B:283:ILE:O	1:B:317:HIS:HA	2.21	0.41
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.73	0.41
1:D:14:ARG:O	1:D:18:GLN:HG3	2.21	0.41
1:D:138:GLU:O	1:D:140:GLU:N	2.54	0.41
1:D:180:THR:HG22	1:D:192:SER:HB3	2.02	0.41
1:A:194:ALA:O	1:A:279:PRO:HA	2.21	0.41
1:C:103:ARG:HA	1:C:147:TYR:HE2	1.86	0.41
1:D:133:ARG:O	1:D:134:LEU:HD12	2.21	0.41
1:A:53:TRP:HB2	1:A:54:PRO:HD2	2.03	0.40
1:B:28:TRP:CD2	1:B:40:PRO:HG2	2.56	0.40
1:B:90:LEU:HB3	1:B:92:LEU:CG	2.49	0.40
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.84	0.40
1:A:84:LYS:HB3	1:A:97:TRP:CE2	2.57	0.40
1:B:84:LYS:NZ	1:B:153:GLU:OE2	2.53	0.40
1:B:288:SER:OG	1:B:343:TYR:OH	2.29	0.40
1:D:10:GLY:N	1:D:49:GLU:OE2	2.51	0.40
1:B:11:GLN:HG3	1:B:305:TYR:CE2	2.56	0.40
1:B:97:TRP:HA	1:B:152:VAL:O	2.21	0.40
1:D:158:PHE:CB	1:D:228:PHE:HB3	2.52	0.40
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.84	0.40
1:C:71:ARG:HH11	1:C:71:ARG:HD3	1.69	0.40
1:C:132:TRP:CD2	1:C:142:LEU:HD12	2.56	0.40
1:C:144:ALA:O	1:C:147:TYR:HD1	2.03	0.40
1:C:293:ASP:O	1:C:296:LYS:HG3	2.21	0.40
1:D:297:LEU:HA	1:D:298:PRO:HD3	1.89	0.40
1:A:96:PRO:O	1:A:153:GLU:HA	2.22	0.40
1:B:332:LEU:O	1:B:335:LEU:HB2	2.22	0.40
1:C:79:ASP:HB3	1:C:82:THR:OG1	2.22	0.40
1:C:245:ASN:HA	1:C:248:HIS:CE1	2.56	0.40
1:C:297:LEU:HA	1:C:298:PRO:HD2	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2439:HOH:O	4:D:2477:HOH:O[1_454]	0.20	2.00

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	347/355 (98%)	329 (95%)	14 (4%)	4 (1%)	13 24
1	B	353/355 (99%)	326 (92%)	21 (6%)	6 (2%)	9 16
1	C	346/355 (98%)	321 (93%)	19 (6%)	6 (2%)	9 16
1	D	346/355 (98%)	331 (96%)	10 (3%)	5 (1%)	11 20
All	All	1392/1420 (98%)	1307 (94%)	64 (5%)	21 (2%)	10 18

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ARG
1	C	146	CYS
1	A	139	THR
1	A	146	CYS
1	C	136	ALA
1	C	140	GLU
1	D	34	ALA
1	D	139	THR
1	A	292	TYR
1	B	139	THR
1	B	104	SER
1	C	104	SER
1	C	113	LEU
1	D	136	ALA
1	A	136	ALA
1	C	139	THR
1	D	40	PRO

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Mol	Chain	Res	Type
1	B	124	GLY
1	B	298	PRO
1	B	125	GLY
1	D	287	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	293/296 (99%)	256 (87%)	37 (13%)	4 8
1	B	296/296 (100%)	248 (84%)	48 (16%)	2 4
1	C	293/296 (99%)	249 (85%)	44 (15%)	3 5
1	D	293/296 (99%)	255 (87%)	38 (13%)	4 7
All	All	1175/1184 (99%)	1008 (86%)	167 (14%)	3 6

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	21	GLU
1	A	23	LEU
1	A	33	ASP
1	A	35	GLU
1	A	42	GLN
1	A	43	GLN
1	A	44	SER
1	A	60	ARG
1	A	68	PHE
1	A	80	ARG
1	A	90	LEU
1	A	98	GLN
1	A	104	SER
1	A	105	GLU
1	A	112	ARG
1	A	118	ILE

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Mol	Chain	Res	Type
1	A	121	ARG
1	A	134	LEU
1	A	149	GLU
1	A	197	GLN
1	A	201	GLN
1	A	209	MET
1	A	215	GLN
1	A	217	LEU
1	A	230	THR
1	A	234	LEU
1	A	239	LEU
1	A	243	VAL
1	A	245	ASN
1	A	306	ASP
1	A	310	ARG
1	A	325	THR
1	A	327	ARG
1	A	336	ILE
1	A	342	GLU
1	A	345	SER
1	B	1	MET
1	B	2	LYS
1	B	9	ASN
1	B	23	LEU
1	B	30	VAL
1	B	32	LEU
1	B	39	VAL
1	B	42	GLN
1	B	43	GLN
1	B	44	SER
1	B	49	GLU
1	B	52	ARG
1	B	61	GLU
1	B	90	LEU
1	B	103	ARG
1	B	104	SER
1	B	111	ASP
1	B	121	ARG
1	B	131	GLN
1	B	134	LEU
1	B	137	ASN
1	B	140	GLU

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	145	GLU
1	B	146	CYS
1	B	152	VAL
1	B	159	SER
1	B	192	SER
1	B	197	GLN
1	B	201	GLN
1	B	211	SER
1	B	230	THR
1	B	232	GLN
1	B	235	LEU
1	B	239	LEU
1	B	245	ASN
1	B	271	LEU
1	B	280	SER
1	B	288	SER
1	B	295	LEU
1	B	306	ASP
1	B	324	ASP
1	B	326	SER
1	B	333	GLU
1	B	337	PRO
1	B	342	GLU
1	B	345	SER
1	B	352	SER
1	C	9	ASN
1	C	33	ASP
1	C	35	GLU
1	C	39	VAL
1	C	42	GLN
1	C	43	GLN
1	C	44	SER
1	C	51	GLU
1	C	60	ARG
1	C	62	LEU
1	C	68	PHE
1	C	71	ARG
1	C	98	GLN
1	C	99	LEU
1	C	102	GLU
1	C	103	ARG

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Mol	Chain	Res	Type
1	C	104	SER
1	C	111	ASP
1	C	112	ARG
1	C	115	GLU
1	C	116	LEU
1	C	131	GLN
1	C	134	LEU
1	C	142	LEU
1	C	146	CYS
1	C	149	GLU
1	C	151	ILE
1	C	152	VAL
1	C	168	ARG
1	C	188	ILE
1	C	192	SER
1	C	196	PRO
1	C	197	GLN
1	C	202	GLN
1	C	211	SER
1	C	235	LEU
1	C	245	ASN
1	C	293	ASP
1	C	296	LYS
1	C	306	ASP
1	C	308	GLU
1	C	327	ARG
1	C	336	ILE
1	C	342	GLU
1	D	9	ASN
1	D	23	LEU
1	D	33	ASP
1	D	36	PRO
1	D	44	SER
1	D	52	ARG
1	D	61	GLU
1	D	68	PHE
1	D	71	ARG
1	D	82	THR
1	D	90	LEU
1	D	103	ARG
1	D	104	SER
1	D	111	ASP

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Mol	Chain	Res	Type
1	D	116	LEU
1	D	123	THR
1	D	131	GLN
1	D	137	ASN
1	D	141	GLN
1	D	145	GLU
1	D	146	CYS
1	D	149	GLU
1	D	175	VAL
1	D	190	ARG
1	D	197	GLN
1	D	211	SER
1	D	215	GLN
1	D	232	GLN
1	D	239	LEU
1	D	245	ASN
1	D	257	SER
1	D	271	LEU
1	D	288	SER
1	D	295	LEU
1	D	306	ASP
1	D	308	GLU
1	D	342	GLU
1	D	345	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	ASN
1	A	42	GLN
1	A	43	GLN
1	A	98	GLN
1	A	182	ASN
1	A	215	GLN
1	B	3	GLN
1	B	9	ASN
1	B	18	GLN
1	B	131	GLN
1	B	182	ASN
1	B	278	ASN
1	B	291	ASN

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Mol	Chain	Res	Type
1	C	9	ASN
1	C	42	GLN
1	C	43	GLN
1	C	98	GLN
1	C	182	ASN
1	D	9	ASN
1	D	18	GLN
1	D	137	ASN
1	D	141	GLN
1	D	182	ASN
1	D	185	GLN
1	D	215	GLN
1	D	301	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	ADP	D	1400	2	24,29,29	1.14	2 (8%)	29,45,45	1.30	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	1100	2	24,29,29	1.13	3 (12%)	29,45,45	1.69	7 (24%)
3	ADP	C	1300	2	24,29,29	1.12	3 (12%)	29,45,45	1.41	5 (17%)
3	ADP	B	1200	2	24,29,29	1.15	3 (12%)	29,45,45	1.32	3 (10%)

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
3	ADP	D	1400	2	-	4/12/32/32	0/3/3/3
3	ADP	A	1100	2	-	4/12/32/32	0/3/3/3
3	ADP	C	1300	2	-	6/12/32/32	0/3/3/3
3	ADP	B	1200	2	-	5/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1100	ADP	O3'-C3'	3.03	1.50	1.43
3	C	1300	ADP	O2'-C2'	2.93	1.49	1.43
3	A	1100	ADP	O2'-C2'	2.89	1.49	1.43
3	B	1200	ADP	O3'-C3'	2.87	1.49	1.43
3	B	1200	ADP	O2'-C2'	2.85	1.49	1.43
3	D	1400	ADP	O2'-C2'	2.80	1.49	1.43
3	C	1300	ADP	C2-N1	2.60	1.38	1.33
3	D	1400	ADP	O3'-C3'	2.57	1.49	1.43
3	A	1100	ADP	C2-N1	2.23	1.38	1.33
3	C	1300	ADP	O3'-C3'	2.07	1.47	1.43
3	B	1200	ADP	O4'-C1'	-2.01	1.38	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1100	ADP	O3'-C3'-C2'	4.68	126.94	111.82
3	C	1300	ADP	O3'-C3'-C2'	4.12	125.17	111.82
3	D	1400	ADP	O3'-C3'-C2'	3.63	123.56	111.82
3	B	1200	ADP	C5-C6-N6	3.43	125.56	120.35
3	A	1100	ADP	C2'-C3'-C4'	-3.41	96.02	102.64
3	A	1100	ADP	O4'-C4'-C3'	-3.31	98.56	105.11
3	B	1200	ADP	C2'-C3'-C4'	-3.28	96.26	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1300	ADP	O2'-C2'-C3'	2.84	121.02	111.82
3	B	1200	ADP	O3'-C3'-C2'	2.73	120.66	111.82
3	A	1100	ADP	O4'-C1'-C2'	-2.56	103.18	106.93
3	D	1400	ADP	C5-C6-N6	2.56	124.24	120.35
3	C	1300	ADP	C5-C6-N1	-2.27	115.21	120.35
3	C	1300	ADP	C2'-C3'-C4'	-2.25	98.27	102.64
3	C	1300	ADP	C4-C5-N7	2.14	111.63	109.40
3	A	1100	ADP	O2'-C2'-C3'	2.14	118.73	111.82
3	D	1400	ADP	O2'-C2'-C3'	2.12	118.69	111.82
3	A	1100	ADP	C4-C5-N7	2.12	111.61	109.40
3	D	1400	ADP	C5-C6-N1	-2.08	115.63	120.35
3	A	1100	ADP	C5-C6-N1	-2.03	115.76	120.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1100	ADP	C5'-O5'-PA-O1A
3	A	1100	ADP	C5'-O5'-PA-O2A
3	A	1100	ADP	C5'-O5'-PA-O3A
3	C	1300	ADP	C5'-O5'-PA-O2A
3	C	1300	ADP	C5'-O5'-PA-O3A
3	D	1400	ADP	PA-O3A-PB-O3B
3	D	1400	ADP	C5'-O5'-PA-O3A
3	A	1100	ADP	O4'-C4'-C5'-O5'
3	B	1200	ADP	O4'-C4'-C5'-O5'
3	B	1200	ADP	C3'-C4'-C5'-O5'
3	C	1300	ADP	O4'-C4'-C5'-O5'
3	D	1400	ADP	O4'-C4'-C5'-O5'
3	B	1200	ADP	PA-O3A-PB-O3B
3	B	1200	ADP	C5'-O5'-PA-O3A
3	B	1200	ADP	C5'-O5'-PA-O2A
3	C	1300	ADP	C5'-O5'-PA-O1A
3	D	1400	ADP	C5'-O5'-PA-O2A
3	C	1300	ADP	PB-O3A-PA-O2A
3	C	1300	ADP	C3'-C4'-C5'-O5'

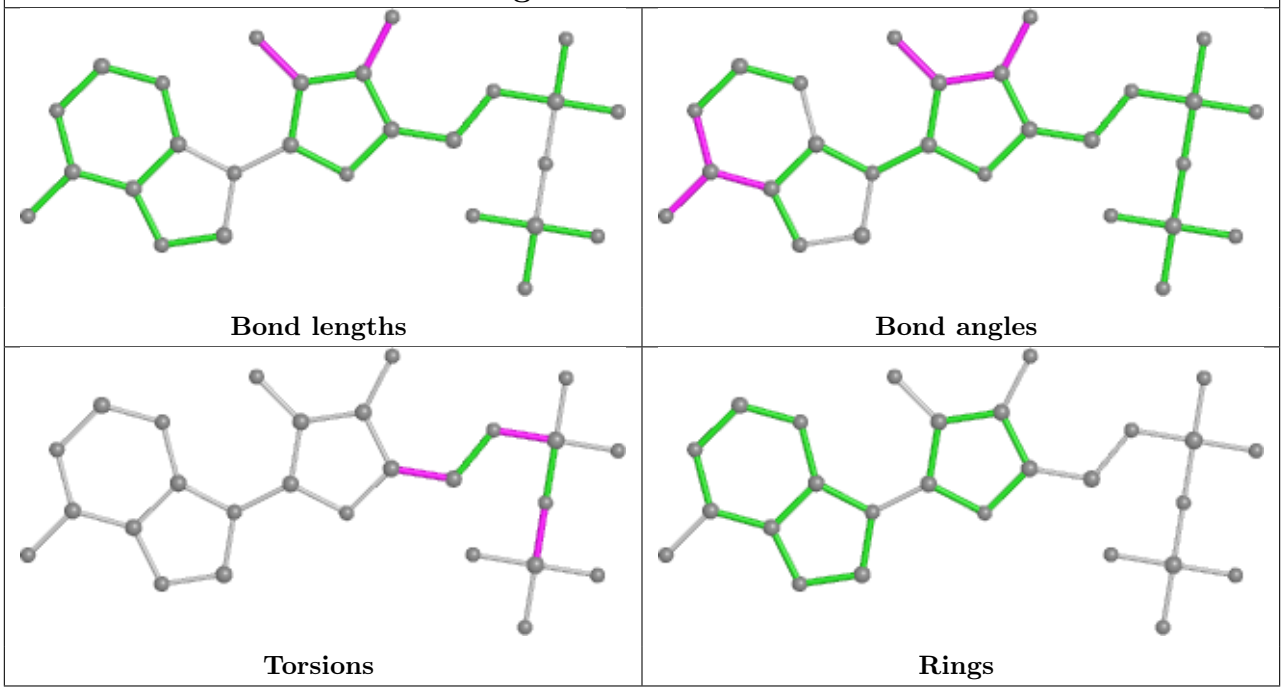
There are no ring outliers.

1 monomer is involved in 1 short contact:

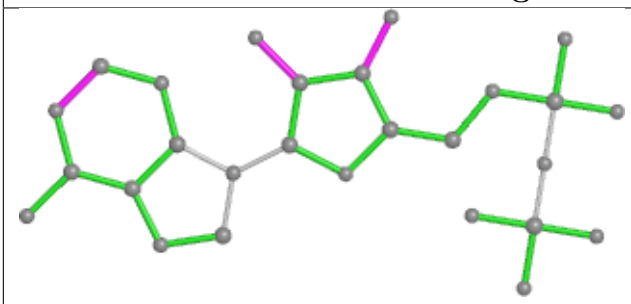
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1200	ADP	1	0

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.

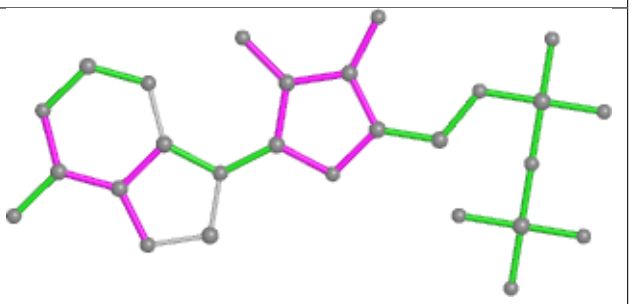
Ligand ADP D 1400



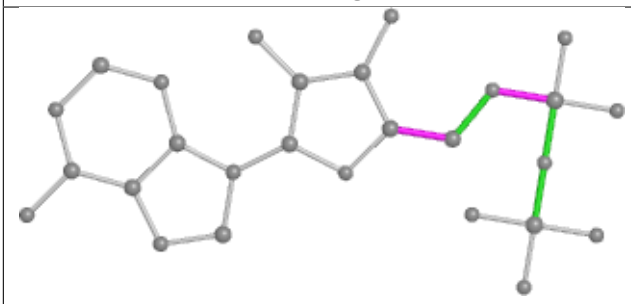
Ligand ADP A 1100



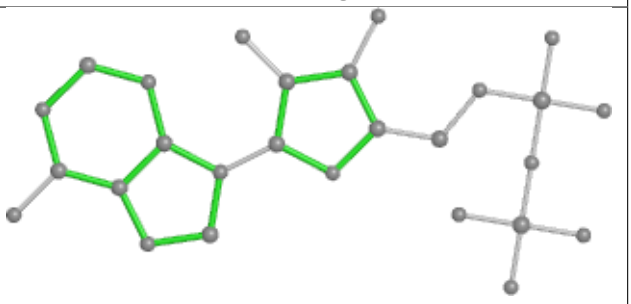
Bond lengths



Bond angles

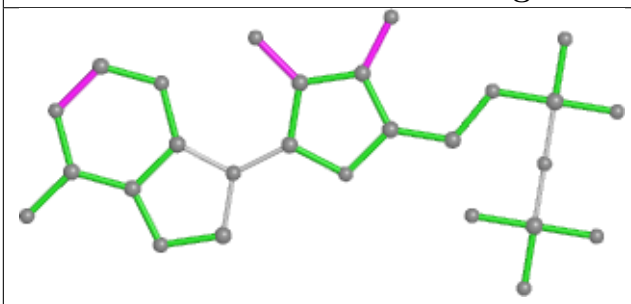


Torsions

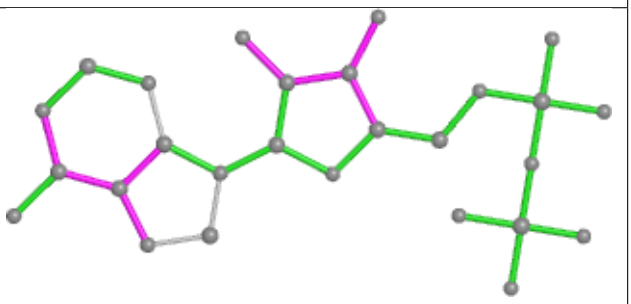


Rings

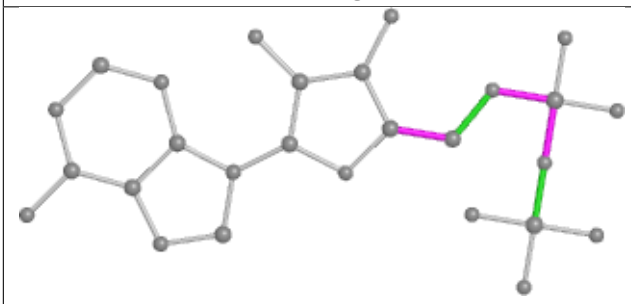
Ligand ADP C 1300



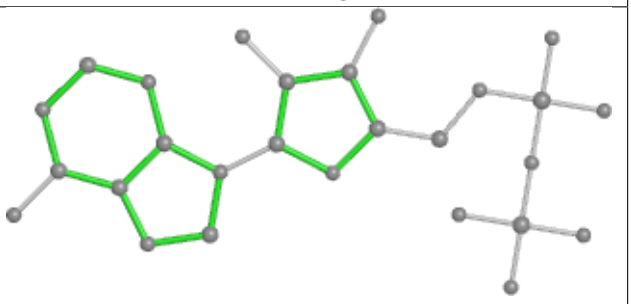
Bond lengths



Bond angles

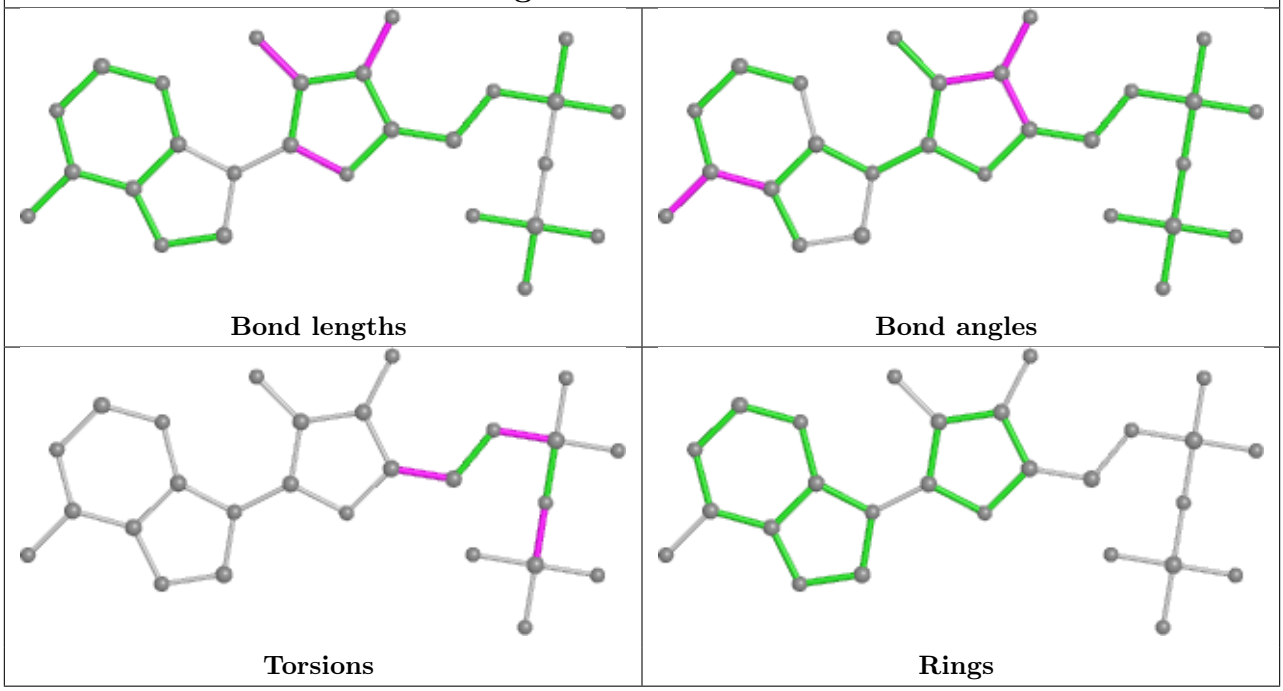


Torsions



Rings

Ligand ADP B 1200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.