



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:28 AM UTC

PDB ID : 1TUG / pdb_00001tug
Title : Aspartate Transcarbamoylase Catalytic Chain Mutant E50A Complex with Phosphonoacetamide, Malonate, and Cytidine-5-Prime-Triphosphate (CTP)
Authors : Stieglitz, K.; Stec, B.; Baker, D.P.; Kantrowitz, E.R.
Deposited on : 2004-06-24
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

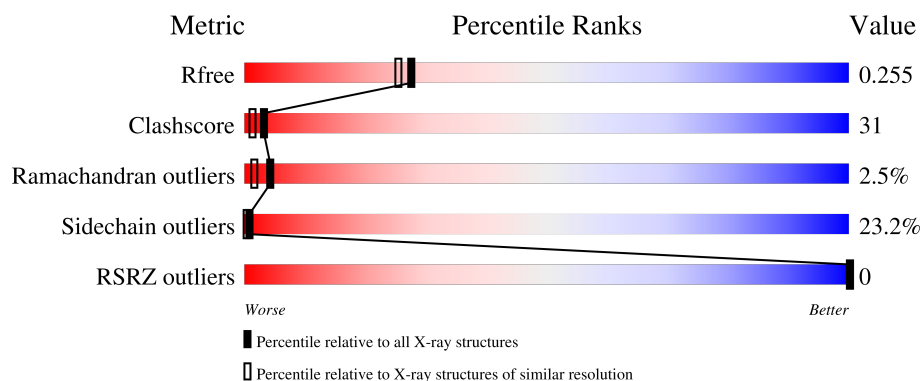
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

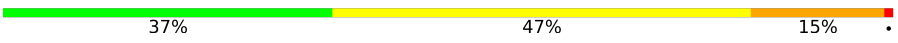
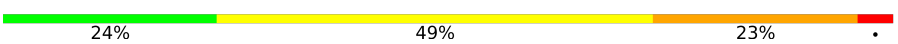
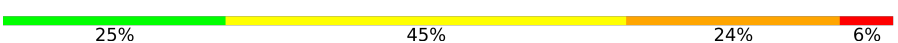
The reported resolution of this entry is 2.10 Å.

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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLI	C	1311	-	-	X	-
4	PCT	C	1313	-	X	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8012 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2411	1525	423	454	9			
1	C	310	Total	C	N	O	S	0	0	0
			2411	1525	423	454	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	ALA	GLU	engineered mutation	UNP P0A786
C	50	ALA	GLU	engineered mutation	UNP P0A786

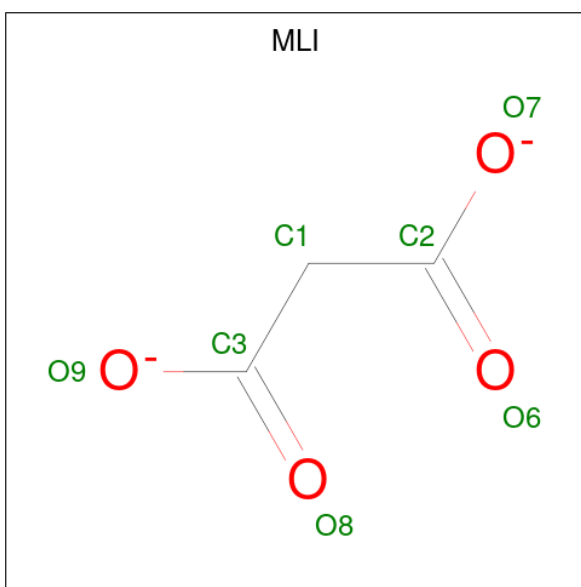
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	D	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

There are 2 discrepancies between the modelled and reference sequences:

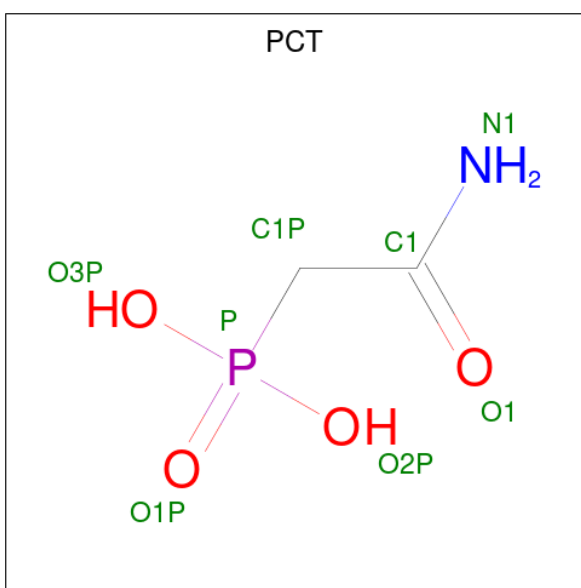
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0A7F3
D	1	MET	-	initiating methionine	UNP P0A7F3

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is PHOSPHONOACETAMIDE (CCD ID: PCT) (formula: C₂H₆NO₄P).

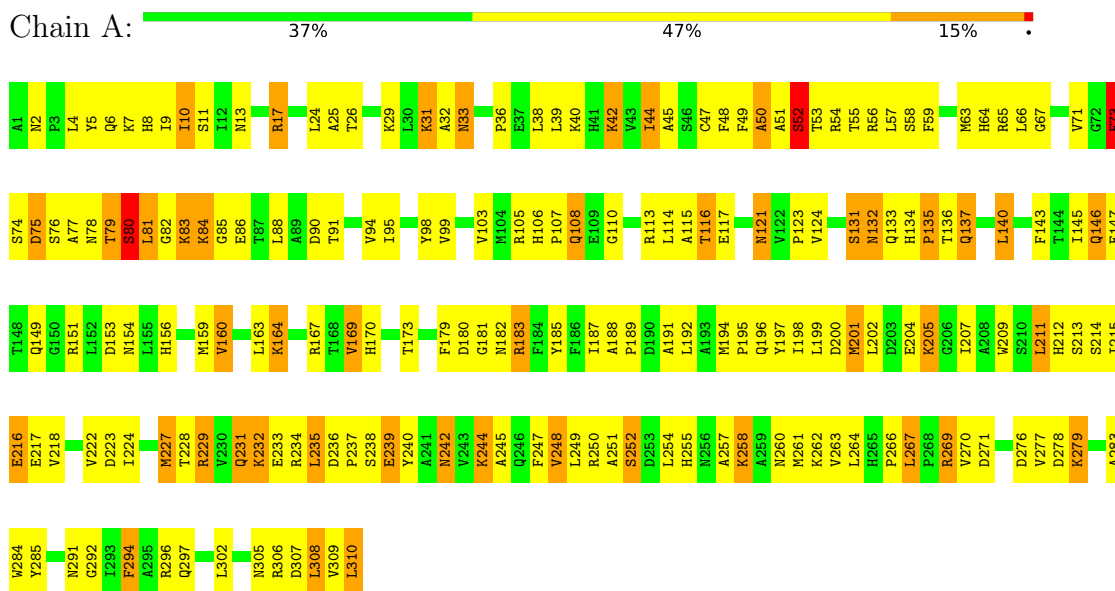


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			8	2	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			8	2	1	4	1		

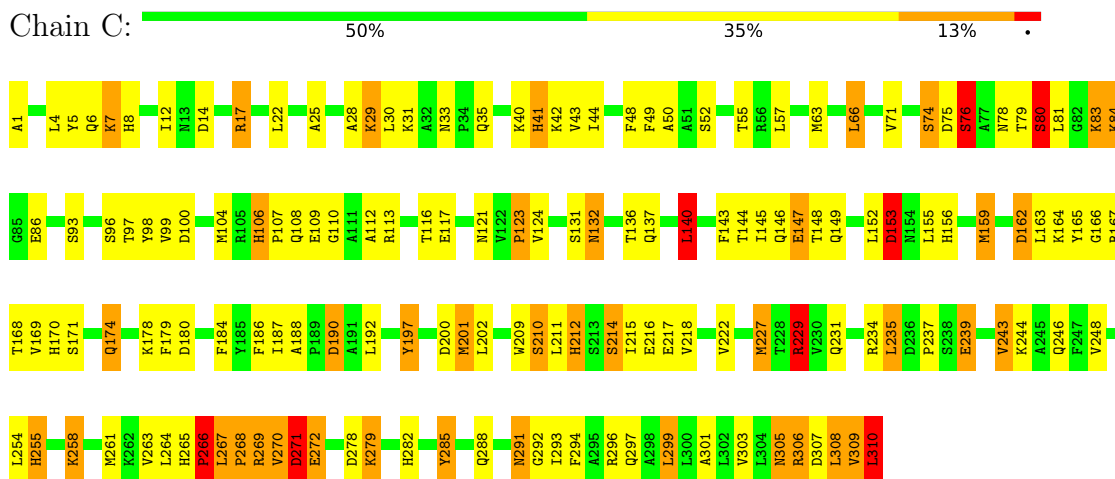
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

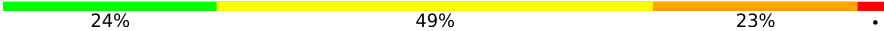
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

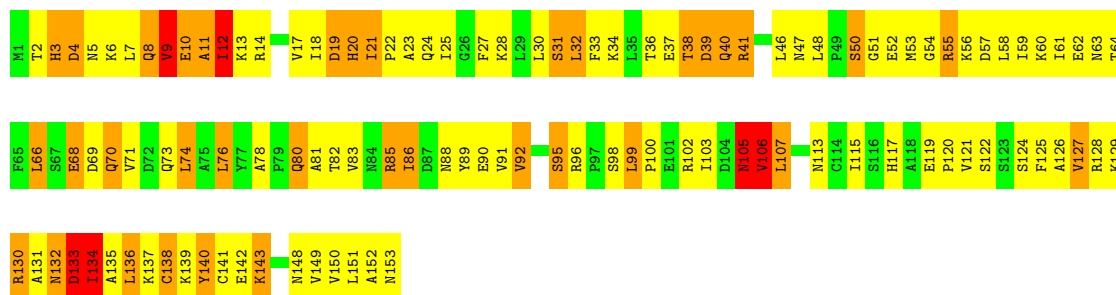


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

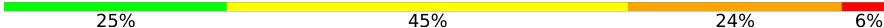


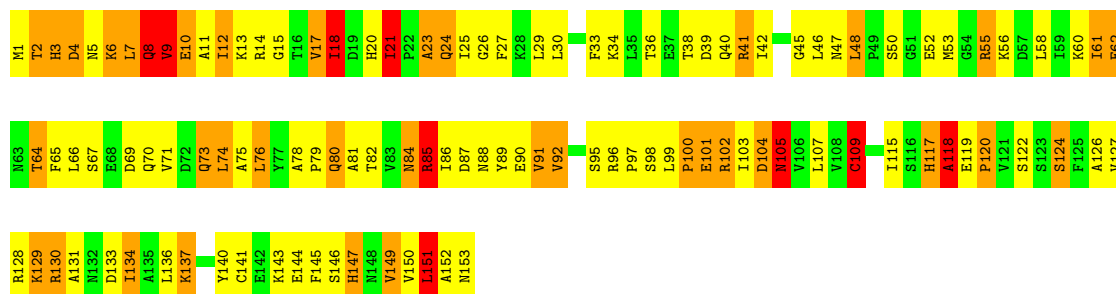
- Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:  24% 49% 23% .



● Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:  25% 45% 24% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.29Å 122.29Å 142.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.1 (30.00-2.10) 92.7 (30.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 2.08Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.230 , 0.272 0.234 , 0.255	Depositor DCC
R_{free} test set	3367 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 376.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8012	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTP, PCT, ZN, MLI

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	1.12	11/2457 (0.4%)	1.80	52/3334 (1.6%)
1	C	1.03	9/2457 (0.4%)	1.75	61/3334 (1.8%)
2	B	1.53	7/1219 (0.6%)	1.71	28/1647 (1.7%)
2	D	1.28	12/1219 (1.0%)	2.04	48/1647 (2.9%)
All	All	1.20	39/7352 (0.5%)	1.81	189/9962 (1.9%)

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	3
1	C	0	4
2	B	0	1
2	D	0	6
All	All	0	14

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	133	ASP	C-N	-34.48	0.86	1.33
1	C	271	ASP	C-N	23.17	1.66	1.34
2	D	8	GLN	C-N	21.87	1.63	1.33
1	A	79	THR	C-N	21.61	1.64	1.33
2	B	134	ILE	C-N	-21.15	1.02	1.33
1	A	80	SER	C-N	20.09	1.63	1.33
1	C	269	ARG	C-N	19.34	1.59	1.33
2	B	20	HIS	C-N	18.04	1.53	1.33
1	A	132	ASN	C-N	17.91	1.57	1.33
1	C	41	HIS	C-N	17.89	1.58	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ALA	C-N	17.76	1.58	1.33
1	A	308	LEU	C-N	17.32	1.57	1.33
1	A	198	ILE	C-N	17.24	1.56	1.33
2	B	152	ALA	C-N	16.29	1.56	1.33
2	D	24	GLN	C-N	16.11	1.55	1.33
1	C	310	LEU	C-OXT	-14.71	0.94	1.23
2	D	153	ASN	C-OXT	14.16	1.51	1.23
1	A	244	LYS	C-N	-13.70	1.14	1.33
2	B	105	ASN	C-N	-12.69	1.16	1.33
1	C	74	SER	C-N	12.66	1.51	1.33
2	B	140	TYR	C-N	11.08	1.49	1.33
2	B	19	ASP	C-N	10.99	1.49	1.33
1	A	269	ARG	C-N	10.19	1.48	1.33
2	D	104	ASP	C-N	-9.69	1.20	1.33
2	D	105	ASN	C-N	-9.26	1.21	1.33
2	D	6	LYS	N-CA	9.10	1.57	1.46
2	D	6	LYS	CA-C	-9.07	1.40	1.52
1	C	267	LEU	C-N	8.87	1.44	1.33
1	C	132	ASN	C-N	8.84	1.45	1.33
2	D	4	ASP	C-N	8.65	1.45	1.33
1	C	76	SER	C-N	8.60	1.44	1.33
1	A	131	SER	C-N	-8.49	1.21	1.33
2	D	6	LYS	C-O	8.38	1.34	1.24
1	A	197	TYR	C-N	-6.42	1.25	1.33
2	D	120	PRO	N-CD	6.36	1.56	1.47
2	D	119	GLU	C-O	-6.16	1.17	1.24
1	C	76	SER	N-CA	5.76	1.53	1.46
1	A	84	LYS	C-N	-5.64	1.25	1.33
2	D	6	LYS	CA-CB	-5.19	1.44	1.53

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	THR	O-C-N	21.20	147.38	123.22
1	A	80	SER	O-C-N	-16.48	100.68	122.59
2	D	105	ASN	O-C-N	-16.40	99.08	122.04
2	D	6	LYS	CB-CA-C	15.88	142.02	110.42
2	D	9	VAL	O-C-N	-14.70	104.20	122.57
2	B	133	ASP	CA-C-N	12.98	145.34	121.97
2	B	133	ASP	C-N-CA	12.98	145.34	121.97
1	C	76	SER	CA-C-O	12.97	139.05	120.51
1	C	267	LEU	CA-C-N	-12.61	106.21	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	C-N-CA	-12.61	106.21	119.83
2	D	104	ASP	O-C-N	-12.29	108.96	123.10
2	B	152	ALA	O-C-N	12.21	134.87	122.30
1	A	84	LYS	O-C-N	11.92	136.03	122.32
2	D	6	LYS	O-C-N	-11.17	107.73	122.59
1	A	269	ARG	O-C-N	-10.95	110.51	123.10
1	A	80	SER	CA-C-N	10.94	142.91	121.58
1	A	80	SER	C-N-CA	10.94	142.91	121.58
1	C	48	PHE	CA-CB-CG	-10.64	103.16	113.80
2	D	4	ASP	O-C-N	10.30	136.29	122.59
2	D	104	ASP	CA-C-N	10.23	140.88	123.91
2	D	104	ASP	C-N-CA	10.23	140.88	123.91
1	C	76	SER	O-C-N	-10.08	109.19	122.59
2	D	24	GLN	O-C-N	-9.91	109.41	122.59
1	A	245	ALA	O-C-N	9.81	135.64	122.59
1	A	79	THR	CA-C-N	-9.59	103.22	121.54
1	A	79	THR	C-N-CA	-9.59	103.22	121.54
2	B	8	GLN	CA-C-N	8.94	132.82	120.49
2	B	8	GLN	C-N-CA	8.94	132.82	120.49
1	C	123	PRO	CA-C-N	8.81	134.57	123.12
1	C	123	PRO	C-N-CA	8.81	134.57	123.12
2	D	85	ARG	CD-NE-CZ	8.62	136.47	124.40
2	D	120	PRO	O-C-N	-8.55	111.09	122.64
2	D	8	GLN	O-C-N	8.51	132.95	123.25
1	C	214	SER	CA-C-N	8.41	131.45	120.60
1	C	214	SER	C-N-CA	8.41	131.45	120.60
2	D	119	GLU	O-C-N	8.39	128.75	121.20
1	A	216	GLU	CA-C-N	8.35	132.57	120.38
1	A	216	GLU	C-N-CA	8.35	132.57	120.38
1	C	40	LYS	CA-C-N	8.32	137.43	121.54
1	C	40	LYS	C-N-CA	8.32	137.43	121.54
1	A	269	ARG	CA-C-N	8.31	131.12	122.97
1	A	269	ARG	C-N-CA	8.31	131.12	122.97
1	C	121	ASN	CA-C-N	-8.15	116.72	122.59
1	C	121	ASN	C-N-CA	-8.15	116.72	122.59
2	D	105	ASN	CA-C-N	-8.14	107.32	121.97
2	D	105	ASN	C-N-CA	-8.14	107.32	121.97
1	A	13	ASN	CA-CB-CG	-8.04	104.56	112.60
2	B	66	LEU	CA-C-N	7.90	134.22	120.87
2	B	66	LEU	C-N-CA	7.90	134.22	120.87
1	C	78	ASN	CA-CB-CG	7.90	120.50	112.60
2	D	6	LYS	CA-C-O	-7.86	109.28	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	23	ALA	CA-C-N	7.71	136.27	121.54
2	D	23	ALA	C-N-CA	7.71	136.27	121.54
1	C	162	ASP	CA-CB-CG	7.57	120.17	112.60
2	B	132	ASN	CA-C-N	-7.53	110.67	122.49
2	B	132	ASN	C-N-CA	-7.53	110.67	122.49
2	D	6	LYS	CA-C-N	7.51	135.88	121.54
2	D	6	LYS	C-N-CA	7.51	135.88	121.54
1	C	106	HIS	CA-CB-CG	7.40	121.20	113.80
1	C	79	THR	CA-C-N	7.38	135.64	121.54
1	C	79	THR	C-N-CA	7.38	135.64	121.54
1	C	80	SER	CA-C-N	7.35	132.78	121.53
1	C	80	SER	C-N-CA	7.35	132.78	121.53
2	B	39	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	83	LYS	O-C-N	-7.31	114.26	122.23
2	D	147	HIS	CA-CB-CG	-7.31	106.49	113.80
1	C	235	LEU	CA-C-N	7.29	133.20	121.83
1	C	235	LEU	C-N-CA	7.29	133.20	121.83
2	B	11	ALA	CA-C-N	7.26	135.04	121.97
2	B	11	ALA	C-N-CA	7.26	135.04	121.97
1	A	76	SER	CA-C-O	7.25	131.99	122.63
1	C	153	ASP	CA-CB-CG	-7.21	105.39	112.60
1	A	48	PHE	CA-CB-CG	-7.16	106.64	113.80
1	A	170	HIS	O-C-N	7.03	129.69	122.09
1	C	79	THR	CA-C-O	6.92	129.29	120.57
2	D	109	CYS	O-C-N	6.88	128.16	121.28
2	D	33	PHE	CA-C-N	6.72	132.37	122.82
2	D	33	PHE	C-N-CA	6.72	132.37	122.82
2	B	117	HIS	CA-CB-CG	-6.70	107.10	113.80
2	D	119	GLU	CA-C-O	6.65	128.25	120.87
1	A	198	ILE	O-C-N	6.64	128.42	121.91
1	C	140	LEU	CA-CB-CG	6.62	139.46	116.30
2	D	117	HIS	CA-CB-CG	6.61	120.41	113.80
1	A	137	GLN	CA-C-O	6.46	127.35	120.70
1	A	294	PHE	CA-CB-CG	-6.42	107.38	113.80
2	D	100	PRO	CA-C-N	6.42	131.28	120.88
2	D	100	PRO	C-N-CA	6.42	131.28	120.88
1	C	106	HIS	CA-C-N	6.32	126.80	119.47
1	C	106	HIS	C-N-CA	6.32	126.80	119.47
1	C	131	SER	O-C-N	-6.32	110.97	122.34
1	A	170	HIS	CA-C-N	6.27	128.68	120.28
1	A	170	HIS	C-N-CA	6.27	128.68	120.28
1	C	146	GLN	OE1-CD-NE2	6.25	128.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	GLN	O-C-N	6.22	126.87	121.34
1	C	268	PRO	CA-N-CD	-6.20	103.33	112.00
1	C	267	LEU	C-N-CD	6.18	150.35	125.00
1	C	255	HIS	CA-CB-CG	-6.16	107.64	113.80
1	C	266	PRO	CA-C-N	6.16	136.83	121.80
1	C	266	PRO	C-N-CA	6.16	136.83	121.80
2	D	18	ILE	CA-C-O	6.12	127.84	120.74
2	B	19	ASP	O-C-N	6.09	131.44	122.97
2	B	9	VAL	CA-C-N	6.08	130.01	121.02
2	B	9	VAL	C-N-CA	6.08	130.01	121.02
1	A	270	VAL	O-C-N	-6.06	117.24	121.85
1	A	188	ALA	N-CA-C	6.06	113.59	108.13
2	D	151	LEU	CA-C-O	6.06	129.18	120.51
1	C	76	SER	CA-C-N	-6.01	114.52	123.00
1	C	76	SER	C-N-CA	-6.01	114.52	123.00
2	D	7	LEU	CA-C-O	6.01	129.10	120.51
1	C	212	HIS	CA-CB-CG	-5.98	107.82	113.80
1	A	308	LEU	O-C-N	-5.96	116.25	123.16
2	D	21	ILE	N-CA-CB	5.95	115.61	110.08
2	D	119	GLU	CA-C-N	-5.95	112.41	119.84
2	D	119	GLU	C-N-CA	-5.95	112.41	119.84
1	C	113	ARG	CD-NE-CZ	5.89	132.65	124.40
2	D	6	LYS	N-CA-CB	-5.87	100.57	110.49
1	A	52	SER	CA-C-N	5.83	132.68	121.54
1	A	52	SER	C-N-CA	5.83	132.68	121.54
1	A	98	TYR	CA-CB-CG	5.83	124.39	113.90
2	B	133	ASP	O-C-N	-5.80	114.67	122.22
1	A	247	PHE	CA-C-N	-5.79	111.94	122.43
1	A	247	PHE	C-N-CA	-5.79	111.94	122.43
1	A	58	SER	CA-C-N	5.78	127.95	120.44
1	A	58	SER	C-N-CA	5.78	127.95	120.44
2	B	125	PHE	CA-CB-CG	-5.74	108.06	113.80
2	D	24	GLN	CA-C-N	5.71	132.25	121.97
2	D	24	GLN	C-N-CA	5.71	132.25	121.97
1	A	115	ALA	CA-C-N	5.71	132.44	121.54
1	A	115	ALA	C-N-CA	5.71	132.44	121.54
2	B	31	SER	CA-C-N	5.70	128.72	120.79
2	B	31	SER	C-N-CA	5.70	128.72	120.79
1	A	103	VAL	CA-C-N	-5.68	113.76	122.62
1	A	103	VAL	C-N-CA	-5.68	113.76	122.62
1	C	71	VAL	CA-C-N	-5.68	113.16	120.72
1	C	71	VAL	C-N-CA	-5.68	113.16	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	VAL	CA-C-N	-5.67	115.23	123.06
1	C	43	VAL	C-N-CA	-5.67	115.23	123.06
2	D	96	ARG	CD-NE-CZ	5.67	132.33	124.40
2	D	120	PRO	CA-N-CD	-5.66	104.07	112.00
1	C	98	TYR	CA-CB-CG	5.64	124.05	113.90
2	D	85	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	44	ILE	CA-C-N	-5.57	114.86	122.93
1	A	44	ILE	C-N-CA	-5.57	114.86	122.93
1	A	50	ALA	CA-C-N	-5.54	112.19	121.39
1	A	50	ALA	C-N-CA	-5.54	112.19	121.39
2	B	151	LEU	CA-C-N	5.53	130.15	121.08
2	B	151	LEU	C-N-CA	5.53	130.15	121.08
2	B	138	CYS	CA-C-N	5.53	127.95	120.38
2	B	138	CYS	C-N-CA	5.53	127.95	120.38
1	C	14	ASP	CA-CB-CG	5.52	118.12	112.60
2	B	134	ILE	O-C-N	-5.51	115.69	122.57
1	A	73	PHE	O-C-N	5.46	129.48	123.25
2	D	62	GLU	CA-C-N	5.45	129.87	122.07
2	D	62	GLU	C-N-CA	5.45	129.87	122.07
1	C	179	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	48	PHE	CA-C-O	5.44	128.02	121.66
2	D	118	ALA	O-C-N	5.37	129.73	122.59
1	A	10	ILE	CA-C-O	5.37	125.58	120.80
1	C	267	LEU	CA-C-O	5.36	127.50	120.16
1	C	156	HIS	CA-CB-CG	-5.35	108.45	113.80
1	A	292	GLY	CA-C-O	5.34	125.80	119.50
1	C	17	ARG	CA-C-O	5.33	126.60	120.90
1	A	33	ASN	CA-C-N	5.32	125.32	119.90
1	A	33	ASN	C-N-CA	5.32	125.32	119.90
1	A	242	ASN	O-C-N	-5.30	116.10	122.15
1	C	184	PHE	CA-CB-CG	-5.29	108.50	113.80
2	D	117	HIS	O-C-N	-5.28	115.57	122.59
2	D	61	ILE	CB-CA-C	-5.28	104.94	111.32
1	A	276	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	99	VAL	CA-C-O	-5.26	116.67	121.72
2	D	6	LYS	CA-CB-CG	5.25	124.60	114.10
1	C	294	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	135	PRO	CA-C-N	5.20	127.24	120.28
1	A	135	PRO	C-N-CA	5.20	127.24	120.28
1	C	237	PRO	CA-C-N	5.19	129.28	120.88
1	C	237	PRO	C-N-CA	5.19	129.28	120.88
1	C	229	ARG	CD-NE-CZ	5.16	131.63	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ASN	CA-CB-CG	-5.15	107.45	112.60
2	B	136	LEU	CA-C-N	-5.14	115.90	123.00
2	B	136	LEU	C-N-CA	-5.14	115.90	123.00
1	C	79	THR	CA-CB-OG1	5.14	117.32	109.60
2	D	7	LEU	O-C-N	-5.13	115.77	122.59
1	A	64	HIS	CA-CB-CG	-5.12	108.68	113.80
1	C	243	VAL	O-C-N	5.09	128.55	122.03
2	D	17	VAL	CA-C-O	5.08	125.67	120.39
1	C	80	SER	N-CA-CB	5.08	119.07	110.49
2	B	133	ASP	CA-C-O	-5.04	113.85	119.95
1	C	202	LEU	CA-C-O	-5.04	115.53	120.82
1	C	197	TYR	CA-CB-CG	5.00	122.91	113.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ASN	Mainchain
1	A	73	PHE	Mainchain
1	A	82	GLY	Mainchain
2	B	133	ASP	Peptide
1	C	266	PRO	Peptide
1	C	269	ARG	Mainchain
1	C	76	SER	Mainchain,Peptide
2	D	105	ASN	Mainchain
2	D	118	ALA	Mainchain
2	D	23	ALA	Mainchain
2	D	5	ASN	Mainchain,Peptide
2	D	9	VAL	Mainchain

5.2 Too-close contacts ⓘ

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	2411	0	2420	155	0
1	C	2411	0	2421	96	0
2	B	1201	0	1216	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1201	0	1219	97	0
3	A	7	0	2	0	0
3	C	7	0	2	4	0
4	A	8	0	4	3	0
4	C	8	0	4	5	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	29	0	12	7	0
6	D	29	0	12	7	0
7	A	211	0	0	26	0
7	B	101	0	0	12	0
7	C	265	0	0	20	0
7	D	121	0	0	14	0
All	All	8012	0	7312	451	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 31.

All (451) 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)
4:C:1313:PCT:H1P2	7:C:1461:HOH:O	1.31	1.25
1:A:67:GLY:HA2	7:A:1510:HOH:O	1.39	1.20
2:B:133:ASP:O	2:B:134:ILE:N	1.78	1.15
1:C:200:ASP:HB3	7:C:1516:HOH:O	1.49	1.11
1:C:234:ARG:NH1	3:C:1311:MLI:H11	1.65	1.11
2:B:133:ASP:C	2:B:134:ILE:CA	2.24	1.09
1:C:234:ARG:HH11	3:C:1311:MLI:H11	0.94	1.07
2:B:133:ASP:CA	2:B:134:ILE:N	2.19	1.06
2:D:131:ALA:HB3	7:D:1272:HOH:O	1.56	1.05
2:D:2:THR:HG21	6:D:1157:CTP:O3'	1.58	1.03
2:D:18:ILE:HG22	2:D:21:ILE:HD11	1.44	0.96
2:D:105:ASN:OD1	2:D:122:SER:HB2	1.64	0.96
2:B:133:ASP:C	2:B:134:ILE:N	0.86	0.96
2:D:17:VAL:HG22	2:D:60:LYS:HG2	1.47	0.96
1:A:235:LEU:HD13	1:A:240:TYR:HB2	1.48	0.95
1:A:26:THR:HA	1:A:29:LYS:HE3	1.49	0.93
2:B:129:LYS:HA	2:B:134:ILE:HG13	1.50	0.93
1:C:267:LEU:HD23	7:C:1474:HOH:O	1.70	0.91
1:C:197:TYR:HD1	7:C:1538:HOH:O	1.55	0.89
2:B:89:TYR:C	6:B:1156:CTP:HN42	1.81	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:HH11	2:B:41:ARG:HB3	1.37	0.88
2:B:38:THR:HG23	2:B:40:GLN:H	1.37	0.88
1:A:73:PHE:HA	7:A:1464:HOH:O	1.76	0.86
1:C:8:HIS:HD2	1:C:124:VAL:H	1.25	0.84
2:B:22:PRO:HB2	2:B:25:ILE:HD13	1.59	0.83
2:B:99:LEU:HD12	2:B:100:PRO:HD2	1.59	0.82
1:A:229:ARG:HH11	1:A:229:ARG:HB3	1.45	0.82
2:D:105:ASN:OD1	2:D:122:SER:CB	2.27	0.81
1:A:32:ALA:HA	7:A:1376:HOH:O	1.80	0.80
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.62	0.78
1:A:252:SER:HB2	7:A:1448:HOH:O	1.84	0.78
2:D:27:PHE:HA	2:D:30:LEU:HD12	1.64	0.78
2:B:18:ILE:HG22	2:B:21:ILE:HD11	1.66	0.77
2:B:85:ARG:HH11	2:B:85:ARG:HB3	1.48	0.77
1:A:81:LEU:HD13	1:A:91:THR:HG23	1.65	0.77
1:A:113:ARG:O	1:A:116:THR:HB	1.85	0.76
2:B:107:LEU:HB2	7:B:1176:HOH:O	1.85	0.76
1:C:254:LEU:HD22	1:C:261:MET:HE1	1.66	0.75
2:D:13:LYS:HD3	7:D:1221:HOH:O	1.85	0.75
1:C:229:ARG:HA	1:C:272:GLU:OE1	1.87	0.75
1:C:265:HIS:H	1:C:288:GLN:HE22	1.35	0.74
2:B:62:GLU:HG2	7:B:1213:HOH:O	1.87	0.74
2:D:41:ARG:HH11	2:D:41:ARG:HB2	1.53	0.74
1:C:234:ARG:NH1	3:C:1311:MLI:C1	2.49	0.74
1:A:231:GLN:O	1:A:234:ARG:HB2	1.87	0.73
2:B:129:LYS:CA	2:B:134:ILE:HG13	2.19	0.73
1:A:191:ALA:O	1:A:192:LEU:HD23	1.88	0.72
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.71	0.71
1:C:174:GLN:HA	1:C:201:MET:HE1	1.71	0.71
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.72	0.71
1:A:51:ALA:HB2	1:A:75:ASP:HB2	1.72	0.71
1:A:81:LEU:HB3	1:A:91:THR:OG1	1.90	0.71
1:C:31:LYS:NZ	1:C:291:ASN:HD21	1.89	0.71
2:D:56:LYS:HE3	2:D:58:LEU:HD12	1.72	0.71
1:A:236:ASP:HB3	1:A:239:GLU:HB3	1.72	0.70
1:A:251:ALA:O	1:A:254:LEU:HB2	1.91	0.70
1:C:266:PRO:HB2	1:C:267:LEU:HG	1.73	0.70
1:C:267:LEU:CD2	7:C:1474:HOH:O	2.32	0.70
1:A:132:ASN:HD22	2:B:143:LYS:HZ1	1.38	0.69
1:A:114:LEU:O	1:A:117:GLU:HG3	1.91	0.69
4:C:1313:PCT:N1	7:C:1474:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASN:HA	1:A:181:GLY:O	1.93	0.69
2:D:17:VAL:HB	2:D:84:ASN:HD22	1.58	0.69
2:D:55:ARG:HH11	2:D:55:ARG:HB3	1.59	0.68
1:A:231:GLN:HB3	1:A:234:ARG:HG3	1.76	0.68
1:A:255:HIS:HB3	7:A:1489:HOH:O	1.93	0.68
1:A:232:LYS:O	1:A:235:LEU:HD12	1.94	0.68
1:A:278:ASP:HB2	1:A:279:LYS:NZ	2.08	0.68
1:A:279:LYS:N	1:A:279:LYS:HE2	2.09	0.67
2:B:38:THR:HG23	2:B:40:GLN:N	2.09	0.67
2:D:102:ARG:HD3	7:D:1215:HOH:O	1.93	0.67
1:C:231:GLN:HB2	1:C:234:ARG:HD2	1.74	0.67
1:A:183:ARG:HH11	1:A:183:ARG:HB3	1.60	0.67
2:B:10:GLU:HA	2:D:8:GLN:NE2	2.09	0.67
2:B:12:ILE:HG13	2:B:86:ILE:HD11	1.76	0.66
1:A:88:LEU:HD23	1:A:114:LEU:HD22	1.77	0.66
1:A:160:VAL:HB	1:A:227:MET:HE3	1.78	0.66
1:A:201:MET:HE3	1:A:202:LEU:N	2.11	0.66
2:B:70:GLN:O	2:B:73:GLN:HB2	1.96	0.66
2:B:89:TYR:O	6:B:1156:CTP:N4	2.25	0.66
2:D:100:PRO:HB2	2:D:101:GLU:OE2	1.96	0.65
2:D:107:LEU:HB2	7:D:1164:HOH:O	1.96	0.65
1:A:74:SER:O	7:A:1454:HOH:O	2.14	0.65
1:C:153:ASP:HB3	1:C:180:ASP:H	1.61	0.65
1:A:154:ASN:HD22	1:A:181:GLY:HA3	1.63	0.64
1:C:234:ARG:HH11	3:C:1311:MLI:C1	1.89	0.64
2:D:25:ILE:O	2:D:29:LEU:HG	1.97	0.64
1:C:52:SER:HA	4:C:1313:PCT:O1P	1.98	0.64
1:A:26:THR:HG23	1:A:308:LEU:HD22	1.79	0.64
2:B:8:GLN:NE2	2:D:9:VAL:O	2.31	0.64
2:B:13:LYS:HG2	7:B:1174:HOH:O	1.98	0.63
2:B:95:SER:HB2	7:B:1177:HOH:O	1.97	0.63
2:B:89:TYR:C	6:B:1156:CTP:N4	2.54	0.63
2:B:76:LEU:HD23	2:B:103:ILE:HD11	1.79	0.63
2:D:45:GLY:HA3	2:D:48:LEU:HD21	1.80	0.63
1:A:235:LEU:HB3	7:A:1484:HOH:O	1.97	0.63
1:A:199:LEU:HD22	1:A:209:TRP:CH2	2.34	0.63
2:B:61:ILE:HG22	2:B:64:THR:HB	1.79	0.63
1:C:279:LYS:HD3	7:C:1390:HOH:O	1.98	0.63
2:B:40:GLN:HG2	2:B:62:GLU:O	1.99	0.62
2:B:48:LEU:O	2:B:55:ARG:HA	1.98	0.62
1:A:235:LEU:HD23	7:A:1484:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ALA:O	1:C:116:THR:HG23	1.99	0.62
2:B:107:LEU:HD13	2:B:150:VAL:HG11	1.80	0.62
2:D:14:ARG:HG3	2:D:87:ASP:HA	1.82	0.62
2:B:10:GLU:HA	2:D:8:GLN:HE22	1.64	0.62
1:A:223:ASP:O	1:A:261:MET:HA	1.99	0.62
1:C:235:LEU:HD22	1:C:239:GLU:OE2	2.00	0.61
1:A:214:SER:O	1:A:217:GLU:HB2	1.99	0.61
2:B:130:ARG:HB2	2:B:133:ASP:HB3	1.82	0.61
1:A:169:VAL:HG23	1:A:194:MET:HE1	1.81	0.61
1:C:145:ILE:O	1:C:149:GLN:HB2	2.01	0.61
2:D:11:ALA:HA	6:D:1157:CTP:N3	2.16	0.61
2:B:14:ARG:HG2	2:B:63:ASN:HA	1.83	0.61
1:C:309:VAL:HG23	7:C:1484:HOH:O	2.00	0.61
2:B:22:PRO:HA	7:B:1194:HOH:O	2.01	0.60
1:A:52:SER:OG	1:A:55:THR:HB	2.01	0.60
2:D:12:ILE:HD12	2:D:14:ARG:O	2.02	0.60
1:A:164:LYS:HG3	7:A:1459:HOH:O	2.02	0.60
2:B:105:ASN:O	2:B:106:VAL:HG13	2.02	0.60
2:D:85:ARG:HD3	2:D:92:VAL:HG23	1.83	0.60
2:D:102:ARG:HH21	2:D:124:SER:HB2	1.67	0.60
2:D:14:ARG:HA	2:D:86:ILE:O	2.02	0.59
1:A:11:SER:HA	1:A:133:GLN:HG3	1.84	0.59
2:B:129:LYS:CB	2:B:134:ILE:HG13	2.31	0.59
1:A:278:ASP:HB2	1:A:279:LYS:HZ1	1.65	0.59
1:A:105:ARG:HH22	4:A:1314:PCT:HN11	1.50	0.59
1:A:232:LYS:HD3	1:A:240:TYR:CZ	2.38	0.59
1:A:131:SER:HB3	7:A:1492:HOH:O	2.01	0.59
1:C:93:SER:O	1:C:97:THR:HG23	2.03	0.59
1:A:182:ASN:O	1:A:207:ILE:HG23	2.03	0.58
2:D:15:GLY:HA2	2:D:64:THR:H	1.68	0.58
2:B:39:ASP:HB2	2:D:55:ARG:HH21	1.69	0.58
2:D:102:ARG:HB3	7:D:1170:HOH:O	2.03	0.58
2:D:79:PRO:HG2	2:D:80:GLN:HG3	1.85	0.58
1:C:166:GLY:O	1:C:169:VAL:HG22	2.03	0.58
2:D:133:ASP:HB3	7:D:1193:HOH:O	2.03	0.58
2:D:38:THR:CG2	2:D:42:ILE:HD11	2.33	0.58
1:A:17:ARG:HD3	1:A:179:PHE:CE1	2.39	0.58
2:B:88:ASN:O	2:B:89:TYR:HB2	2.03	0.58
1:C:22:LEU:HB2	7:C:1553:HOH:O	2.04	0.58
1:C:168:THR:HG23	7:C:1369:HOH:O	2.04	0.57
1:C:5:TYR:CE1	1:C:6:GLN:HG2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:HG13	1:C:271:ASP:O	2.04	0.57
2:B:21:ILE:HB	2:B:57:ASP:HB2	1.85	0.57
2:B:130:ARG:CG	2:B:133:ASP:HB3	2.35	0.57
1:C:50:ALA:HB2	1:C:107:PRO:HD3	1.86	0.57
1:C:258:LYS:HB3	7:C:1535:HOH:O	2.05	0.57
2:D:11:ALA:HA	6:D:1157:CTP:O2	2.05	0.57
1:A:194:MET:SD	1:A:195:PRO:HD2	2.45	0.57
1:A:132:ASN:HD22	2:B:143:LYS:NZ	2.02	0.56
2:B:4:ASP:OD1	2:B:9:VAL:HG21	2.04	0.56
1:A:81:LEU:HD23	1:A:86:GLU:OE1	2.05	0.56
2:B:69:ASP:O	2:B:73:GLN:HG2	2.05	0.56
2:D:2:THR:CG2	6:D:1157:CTP:O3'	2.41	0.56
2:D:10:GLU:HA	2:D:10:GLU:OE1	2.05	0.56
2:B:129:LYS:HA	2:B:134:ILE:HA	1.88	0.56
2:D:78:ALA:HB1	2:D:81:ALA:HB2	1.87	0.56
1:A:59:PHE:HZ	1:A:136:THR:HG21	1.71	0.56
1:A:183:ARG:HH11	1:A:183:ARG:CB	2.19	0.56
1:A:205:LYS:HB2	1:A:205:LYS:NZ	2.20	0.56
1:A:11:SER:HB2	1:A:133:GLN:HG3	1.86	0.56
2:B:30:LEU:HD21	2:B:59:ILE:HD13	1.88	0.56
2:B:107:LEU:HD13	2:B:150:VAL:CG1	2.36	0.56
1:A:33:ASN:HB3	7:A:1418:HOH:O	2.05	0.55
1:A:163:LEU:O	1:A:195:PRO:HD3	2.07	0.55
1:A:159:MET:HE1	1:A:173:THR:OG1	2.06	0.55
1:C:1:ALA:HB2	1:C:306:ARG:HD3	1.87	0.55
2:D:127:VAL:HG22	2:D:136:LEU:CD2	2.36	0.55
2:D:11:ALA:HA	6:D:1157:CTP:C2	2.42	0.55
1:A:187:ILE:HG13	1:A:212:HIS:HB2	1.89	0.55
1:A:257:ALA:HB1	1:A:261:MET:HE3	1.88	0.55
2:B:10:GLU:HG2	7:B:1239:HOH:O	2.07	0.55
1:A:50:ALA:HB3	1:A:105:ARG:HG2	1.88	0.55
1:C:270:VAL:O	1:C:272:GLU:N	2.40	0.55
2:D:8:GLN:NE2	2:D:8:GLN:HA	2.21	0.55
2:B:78:ALA:HB1	2:B:81:ALA:HB2	1.88	0.55
1:C:8:HIS:CD2	1:C:123:PRO:HA	2.42	0.55
1:A:239:GLU:HA	7:A:1393:HOH:O	2.07	0.55
2:B:13:LYS:HG3	2:B:14:ARG:N	2.21	0.55
2:D:126:ALA:O	2:D:136:LEU:HA	2.06	0.55
1:C:165:TYR:CD2	1:C:234:ARG:HD3	2.42	0.54
2:B:130:ARG:CB	2:B:133:ASP:HB3	2.38	0.54
1:A:8:HIS:CD2	7:A:1508:HOH:O	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HD13	1:A:63:MET:HG2	1.90	0.54
1:A:90:ASP:O	1:A:94:VAL:HG23	2.07	0.54
1:A:169:VAL:CG1	1:A:228:THR:HG21	2.38	0.54
1:C:31:LYS:HZ2	1:C:291:ASN:HD21	1.54	0.54
2:B:17:VAL:HG22	2:B:60:LYS:CG	2.37	0.54
2:D:103:ILE:HG13	2:D:127:VAL:HG21	1.90	0.54
1:A:216:GLU:HG2	7:A:1451:HOH:O	2.07	0.54
1:A:258:LYS:HD3	7:A:1379:HOH:O	2.07	0.53
2:B:129:LYS:O	2:B:129:LYS:HG3	2.06	0.53
4:C:1313:PCT:N1	7:C:1398:HOH:O	2.31	0.53
2:D:73:GLN:HA	2:D:73:GLN:OE1	2.07	0.53
1:C:282:HIS:HA	7:C:1462:HOH:O	2.07	0.53
1:C:44:ILE:HG21	1:C:63:MET:HE2	1.91	0.53
2:B:50:SER:HB3	2:B:54:GLY:C	2.34	0.53
2:B:86:ILE:HD13	6:B:1156:CTP:C4	2.44	0.53
1:C:30:LEU:HD23	7:C:1482:HOH:O	2.09	0.53
2:D:102:ARG:HH21	2:D:124:SER:CB	2.21	0.53
2:B:130:ARG:NE	2:B:135:ALA:HB2	2.24	0.52
1:A:31:LYS:NZ	1:A:291:ASN:HD21	2.07	0.52
1:C:254:LEU:HD22	1:C:261:MET:CE	2.37	0.52
1:A:231:GLN:HA	7:A:1498:HOH:O	2.09	0.52
1:A:121:ASN:HA	7:A:1321:HOH:O	2.09	0.52
2:B:141:CYS:O	2:B:143:LYS:HE2	2.09	0.52
2:D:137:LYS:HE3	7:D:1171:HOH:O	2.10	0.52
1:C:55:THR:OG1	4:C:1313:PCT:O1	2.26	0.52
1:C:31:LYS:HZ1	1:C:291:ASN:HD21	1.57	0.52
2:B:76:LEU:HD23	2:B:103:ILE:CD1	2.40	0.52
1:C:165:TYR:HD2	1:C:234:ARG:HD3	1.74	0.52
1:C:187:ILE:HG12	1:C:212:HIS:HB2	1.92	0.52
1:A:47:CYS:HB3	1:A:49:PHE:CE1	2.45	0.51
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.45	0.51
1:A:121:ASN:HB3	7:A:1321:HOH:O	2.08	0.51
2:D:10:GLU:HB3	7:D:1275:HOH:O	2.10	0.51
2:D:146:SER:O	2:D:149:VAL:HG13	2.10	0.51
1:A:110:GLY:HA3	2:B:140:TYR:HB3	1.92	0.51
2:B:13:LYS:HG3	2:B:14:ARG:H	1.76	0.51
1:A:11:SER:CB	1:A:133:GLN:HG3	2.41	0.51
1:A:229:ARG:HH11	1:A:229:ARG:CB	2.21	0.51
2:D:55:ARG:HH11	2:D:55:ARG:CB	2.23	0.50
1:A:187:ILE:HA	1:A:212:HIS:O	2.11	0.50
1:A:105:ARG:HD3	7:A:1427:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:HIS:O	2:B:9:VAL:HG23	2.11	0.50
1:C:7:LYS:HA	7:C:1549:HOH:O	2.12	0.50
1:A:31:LYS:HG3	1:A:294:PHE:CD2	2.46	0.50
1:A:45:ALA:HA	1:A:71:VAL:O	2.12	0.50
2:B:27:PHE:HD2	7:D:1172:HOH:O	1.94	0.50
1:A:223:ASP:O	1:A:224:ILE:HD13	2.12	0.50
2:B:80:GLN:HA	2:B:80:GLN:NE2	2.21	0.50
2:D:41:ARG:HB2	2:D:41:ARG:NH1	2.23	0.50
2:D:78:ALA:O	2:D:97:PRO:HG3	2.12	0.50
1:A:199:LEU:HD22	1:A:209:TRP:CZ3	2.47	0.49
1:C:49:PHE:CE1	1:C:104:MET:HE3	2.47	0.49
1:A:244:LYS:HG3	1:A:248:VAL:HG12	1.95	0.49
2:B:133:ASP:O	2:B:133:ASP:OD2	2.30	0.49
2:D:91:VAL:O	2:D:91:VAL:HG22	2.11	0.49
1:A:4:LEU:O	1:A:7:LYS:HB2	2.12	0.49
1:C:263:VAL:C	1:C:264:LEU:HD23	2.37	0.49
1:C:301:ALA:O	1:C:305:ASN:HB2	2.12	0.49
2:B:126:ALA:O	2:B:136:LEU:HA	2.12	0.49
1:C:136:THR:HG22	1:C:299:LEU:CD2	2.43	0.49
1:C:144:THR:O	1:C:148:THR:HG23	2.12	0.49
1:A:218:VAL:O	1:A:222:VAL:HG13	2.12	0.48
2:D:101:GLU:HB2	7:D:1170:HOH:O	2.13	0.48
2:D:104:ASP:OD2	2:D:124:SER:HB2	2.13	0.48
1:A:236:ASP:N	1:A:239:GLU:HG2	2.28	0.48
2:D:145:PHE:HB2	2:D:150:VAL:HG22	1.95	0.48
1:A:121:ASN:HA	7:A:1487:HOH:O	2.13	0.48
2:B:8:GLN:HE21	2:D:10:GLU:HA	1.79	0.48
2:B:115:ILE:HG13	2:B:115:ILE:O	2.13	0.48
1:C:308:LEU:HB3	1:C:310:LEU:HD22	1.94	0.48
1:A:52:SER:OG	1:A:52:SER:O	2.30	0.48
1:A:263:VAL:C	1:A:264:LEU:HD23	2.39	0.48
1:C:164:LYS:HE2	1:C:165:TYR:CZ	2.49	0.48
1:A:236:ASP:HB3	1:A:239:GLU:CB	2.43	0.48
1:C:265:HIS:ND1	1:C:266:PRO:HD2	2.28	0.48
1:C:293:ILE:O	1:C:297:GLN:HG3	2.14	0.48
1:A:136:THR:HB	1:A:296:ARG:HE	1.78	0.48
2:B:96:ARG:NH1	2:B:96:ARG:HB3	2.28	0.48
2:D:67:SER:OG	2:D:70:GLN:HG3	2.14	0.48
2:B:71:VAL:O	2:B:74:LEU:HG	2.14	0.47
1:A:164:LYS:HB2	1:A:192:LEU:C	2.39	0.47
1:A:8:HIS:CE1	1:A:123:PRO:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD22	1:A:143:PHE:HB2	1.97	0.47
1:A:80:SER:HA	1:A:84:LYS:HB2	1.95	0.47
1:A:156:HIS:HB3	1:A:185:TYR:HE1	1.78	0.47
2:D:20:HIS:HD2	2:D:82:THR:HG23	1.78	0.47
1:A:227:MET:HB3	1:A:227:MET:HE2	1.68	0.47
2:B:50:SER:HB3	2:B:54:GLY:O	2.14	0.47
2:D:109:CYS:O	2:D:117:HIS:CE1	2.68	0.47
1:A:29:LYS:HB3	1:A:310:LEU:HD22	1.96	0.47
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.49	0.47
1:A:306:ARG:HG2	7:A:1429:HOH:O	2.13	0.47
6:B:1156:CTP:O2B	6:B:1156:CTP:O3G	2.33	0.47
1:C:159:MET:HG3	1:C:186:PHE:CE1	2.50	0.47
2:D:136:LEU:HD12	2:D:147:HIS:HA	1.97	0.47
2:B:107:LEU:CD1	2:B:136:LEU:HD13	2.45	0.47
2:B:121:VAL:HB	2:B:140:TYR:OH	2.15	0.47
2:D:3:HIS:O	2:D:4:ASP:HB2	2.15	0.47
2:D:50:SER:O	2:D:50:SER:OG	2.29	0.47
1:A:25:ALA:HB2	7:A:1479:HOH:O	2.15	0.47
1:A:145:ILE:HG12	1:A:224:ILE:HG13	1.96	0.47
1:C:152:LEU:HA	1:C:155:LEU:HD11	1.97	0.46
2:D:21:ILE:HD13	2:D:21:ILE:N	2.30	0.46
2:D:145:PHE:HB2	2:D:150:VAL:CG2	2.45	0.46
1:C:137:GLN:HA	1:C:140:LEU:HD13	1.97	0.46
1:C:210:SER:C	1:C:211:LEU:HD23	2.40	0.46
1:A:232:LYS:H	1:A:232:LYS:HG2	1.38	0.46
2:B:76:LEU:HD13	2:B:76:LEU:HA	1.66	0.46
1:C:5:TYR:CD2	1:C:306:ARG:HA	2.51	0.46
2:D:11:ALA:CA	6:D:1157:CTP:N3	2.79	0.46
2:D:67:SER:O	2:D:71:VAL:HG23	2.15	0.46
1:A:11:SER:CA	1:A:133:GLN:HG3	2.46	0.46
2:B:86:ILE:HD13	6:B:1156:CTP:N3	2.31	0.46
1:C:110:GLY:HA3	2:D:140:TYR:HB3	1.96	0.46
2:B:8:GLN:NE2	2:D:10:GLU:HA	2.31	0.46
1:C:42:LYS:HA	1:C:100:ASP:OD2	2.16	0.46
2:B:8:GLN:HB3	2:D:10:GLU:HG2	1.98	0.46
2:B:50:SER:N	2:B:54:GLY:O	2.49	0.46
2:D:99:LEU:CD1	2:D:134:ILE:HD12	2.46	0.46
2:B:47:ASN:OD1	2:B:55:ARG:NH1	2.49	0.46
1:C:83:LYS:H	1:C:83:LYS:HG2	1.43	0.46
2:B:124:SER:HB3	2:B:139:LYS:HD2	1.97	0.45
1:A:134:HIS:CD2	4:A:1314:PCT:HN12	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:NH2	1:A:180:ASP:OD1	2.50	0.45
1:A:153:ASP:OD1	1:A:179:PHE:HB3	2.17	0.45
2:B:23:ALA:O	2:B:24:GLN:HB2	2.15	0.45
2:D:73:GLN:NE2	7:D:1173:HOH:O	2.50	0.45
2:D:144:GLU:HB3	7:D:1252:HOH:O	2.16	0.45
1:A:9:ILE:C	1:A:10:ILE:HD13	2.42	0.45
1:A:234:ARG:NE	7:A:1525:HOH:O	2.50	0.45
1:A:277:VAL:O	1:A:283:ALA:HB2	2.17	0.45
1:C:30:LEU:HA	7:C:1482:HOH:O	2.17	0.45
2:D:102:ARG:NE	2:D:104:ASP:OD2	2.49	0.45
2:B:2:THR:O	2:B:4:ASP:N	2.50	0.45
2:B:41:ARG:NH1	2:B:62:GLU:OE2	2.50	0.45
2:B:138:CYS:O	2:B:142:GLU:HA	2.17	0.45
2:B:153:ASN:C	7:B:1232:HOH:O	2.59	0.45
1:C:255:HIS:CD2	1:C:255:HIS:H	2.34	0.45
1:C:291:ASN:HD22	1:C:291:ASN:HA	1.50	0.45
1:A:56:ARG:NH1	7:A:1482:HOH:O	2.50	0.45
2:B:128:ARG:O	2:B:135:ALA:N	2.49	0.45
1:C:7:LYS:NZ	7:C:1375:HOH:O	2.49	0.45
1:A:209:TRP:HZ3	1:A:211:LEU:HD21	1.81	0.45
2:B:22:PRO:HG3	7:B:1175:HOH:O	2.16	0.45
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.32	0.45
2:B:127:VAL:O	2:B:127:VAL:HG12	2.17	0.45
1:C:267:LEU:HB3	1:C:268:PRO:HD2	1.97	0.45
1:A:205:LYS:HB2	1:A:205:LYS:HZ3	1.81	0.45
1:C:84:LYS:O	1:C:84:LYS:HG3	2.17	0.45
1:A:137:GLN:OE1	1:A:140:LEU:HD22	2.16	0.45
1:A:232:LYS:HA	1:A:235:LEU:HD11	1.99	0.45
2:B:32:LEU:HD23	2:B:106:VAL:CG1	2.47	0.45
2:B:131:ALA:O	2:B:132:ASN:HB3	2.17	0.44
2:D:80:GLN:HE21	2:D:80:GLN:C	2.25	0.44
1:A:258:LYS:HB3	1:A:260:ASN:OD1	2.16	0.44
1:A:266:PRO:O	1:A:267:LEU:HB2	2.17	0.44
2:B:148:ASN:HA	7:B:1199:HOH:O	2.16	0.44
2:D:48:LEU:O	2:D:56:LYS:N	2.49	0.44
1:A:169:VAL:CG2	1:A:194:MET:HE1	2.47	0.44
1:A:257:ALA:CB	1:A:261:MET:HE3	2.47	0.44
2:D:2:THR:CB	6:D:1157:CTP:O2B	2.65	0.44
2:D:101:GLU:OE2	2:D:101:GLU:N	2.50	0.44
2:B:46:LEU:HB2	2:D:42:ILE:HB	1.98	0.44
1:A:66:LEU:HD21	1:A:297:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:VAL:C	1:C:272:GLU:H	2.25	0.44
2:D:14:ARG:CG	2:D:87:ASP:HA	2.47	0.44
2:D:17:VAL:CB	2:D:84:ASN:HD22	2.29	0.44
2:D:115:ILE:C	2:D:117:HIS:H	2.25	0.44
1:C:25:ALA:O	1:C:28:ALA:HB3	2.18	0.44
1:C:109:GLU:HG2	1:C:132:ASN:HB2	1.99	0.44
1:C:170:HIS:O	1:C:174:GLN:HG3	2.16	0.44
2:D:103:ILE:HG13	2:D:127:VAL:CG2	2.46	0.44
1:A:236:ASP:HB3	1:A:239:GLU:HG2	1.99	0.44
2:B:80:GLN:HB2	7:B:1175:HOH:O	2.16	0.44
1:C:143:PHE:O	1:C:147:GLU:HB3	2.18	0.44
1:C:305:ASN:ND2	7:C:1410:HOH:O	2.50	0.44
2:D:26:GLY:O	2:D:30:LEU:HG	2.17	0.43
2:D:137:LYS:HD2	7:D:1171:HOH:O	2.18	0.43
2:B:10:GLU:H	2:B:10:GLU:HG3	1.36	0.43
2:B:96:ARG:HB3	2:B:96:ARG:HH11	1.84	0.43
1:C:278:ASP:OD2	1:C:285:TYR:OH	2.32	0.43
2:B:34:LYS:NZ	7:B:1165:HOH:O	2.50	0.43
2:B:36:THR:O	2:B:38:THR:N	2.50	0.43
1:A:236:ASP:OD2	1:A:239:GLU:HB3	2.18	0.43
2:B:71:VAL:HG22	2:B:83:VAL:HG21	1.99	0.43
2:B:86:ILE:HG22	2:B:91:VAL:HA	1.99	0.43
1:C:299:LEU:HD12	1:C:299:LEU:HA	1.54	0.43
2:D:38:THR:HG21	2:D:42:ILE:HD11	1.99	0.43
2:B:85:ARG:O	2:B:92:VAL:HG23	2.18	0.43
1:C:200:ASP:CB	7:C:1516:HOH:O	2.30	0.43
1:A:77:ALA:O	1:A:83:LYS:HD3	2.19	0.43
1:A:146:GLN:HG3	1:A:147:GLU:N	2.27	0.43
2:B:14:ARG:HG2	2:B:63:ASN:HD22	1.84	0.43
2:B:27:PHE:CD1	2:D:36:THR:HG21	2.53	0.43
1:C:162:ASP:OD2	1:C:192:LEU:HD22	2.18	0.43
1:C:285:TYR:HA	1:C:288:GLN:HE21	1.82	0.43
1:A:145:ILE:HG22	1:A:146:GLN:N	2.33	0.43
1:A:222:VAL:HG23	1:A:261:MET:HG3	2.01	0.43
1:A:232:LYS:HD3	1:A:240:TYR:OH	2.19	0.43
1:A:306:ARG:HG3	1:A:307:ASP:CG	2.43	0.43
1:A:26:THR:HG23	1:A:308:LEU:CD2	2.48	0.43
2:B:28:LYS:O	2:B:32:LEU:HB2	2.19	0.43
1:A:105:ARG:HD3	1:A:105:ARG:HH11	1.63	0.42
1:A:196:GLN:HE21	1:A:200:ASP:CG	2.26	0.42
1:A:196:GLN:NE2	1:A:200:ASP:OD1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ILE:HD13	2:B:21:ILE:N	2.34	0.42
1:C:29:LYS:HG2	7:C:1491:HOH:O	2.18	0.42
1:A:134:HIS:N	1:A:135:PRO:HD3	2.34	0.42
2:B:68:GLU:H	2:B:68:GLU:HG3	1.66	0.42
1:A:54:ARG:HB3	4:A:1314:PCT:O2P	2.19	0.42
1:A:2:ASN:ND2	1:A:5:TYR:HB2	2.34	0.42
1:A:65:ARG:NE	7:A:1512:HOH:O	2.50	0.42
1:A:236:ASP:HB3	1:A:239:GLU:CG	2.50	0.42
1:A:36:PRO:HA	1:A:65:ARG:O	2.19	0.42
1:A:54:ARG:HB2	1:A:54:ARG:NH1	2.34	0.42
1:C:4:LEU:HD23	1:C:4:LEU:HA	1.88	0.42
1:C:66:LEU:HD12	1:C:66:LEU:HA	1.89	0.42
1:C:261:MET:HE3	1:C:282:HIS:ND1	2.35	0.42
2:D:71:VAL:HA	2:D:74:LEU:CD1	2.50	0.42
1:C:209:TRP:CZ3	1:C:211:LEU:HD21	2.54	0.42
2:D:133:ASP:HB2	2:D:147:HIS:HE1	1.84	0.42
2:D:76:LEU:HD23	2:D:151:LEU:HD21	2.00	0.42
1:C:263:VAL:O	1:C:264:LEU:HD23	2.19	0.42
2:D:150:VAL:C	2:D:152:ALA:H	2.28	0.42
1:A:258:LYS:HZ2	1:A:258:LYS:HG2	1.65	0.41
2:B:19:ASP:OD1	2:B:20:HIS:N	2.50	0.41
1:A:17:ARG:HB3	7:A:1399:HOH:O	2.19	0.41
1:A:262:LYS:HD2	1:A:284:TRP:CD2	2.56	0.41
1:A:39:LEU:HD22	1:A:42:LYS:HD2	2.02	0.41
2:B:80:GLN:OE1	2:B:96:ARG:NH2	2.50	0.41
1:A:235:LEU:HB2	1:A:239:GLU:CG	2.51	0.41
2:B:119:GLU:HB3	2:B:120:PRO:HD2	2.03	0.41
1:C:218:VAL:O	1:C:222:VAL:HG13	2.20	0.41
2:D:65:PHE:C	2:D:66:LEU:HD23	2.45	0.41
1:C:106:HIS:CE1	1:C:107:PRO:HG2	2.55	0.41
1:A:33:ASN:O	1:A:310:LEU:HD21	2.19	0.41
2:B:11:ALA:O	6:B:1156:CTP:O2	2.38	0.41
2:D:65:PHE:HA	7:D:1207:HOH:O	2.19	0.41
1:C:190:ASP:OD1	1:C:190:ASP:N	2.50	0.41
2:D:115:ILE:O	2:D:115:ILE:HG13	2.21	0.41
2:D:129:LYS:HZ3	2:D:129:LYS:HG2	1.77	0.41
1:A:77:ALA:O	1:A:83:LYS:CD	2.68	0.41
1:C:214:SER:O	1:C:217:GLU:HG3	2.21	0.41
1:A:236:ASP:HA	1:A:237:PRO:HD2	1.91	0.41
1:A:271:ASP:N	1:A:271:ASP:OD2	2.53	0.41
1:A:45:ALA:HB2	1:A:99:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ILE:O	1:A:95:ILE:HG22	2.20	0.41
2:D:88:ASN:O	2:D:90:GLU:N	2.54	0.41
2:B:33:PHE:CE2	2:B:73:GLN:HB3	2.56	0.40
1:C:153:ASP:HB2	1:C:180:ASP:O	2.21	0.40
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.85	0.40
2:D:46:LEU:O	2:D:47:ASN:HB2	2.20	0.40
2:B:41:ARG:HH11	2:B:41:ARG:CB	2.20	0.40
1:C:308:LEU:HD13	1:C:308:LEU:HA	1.81	0.40
1:A:2:ASN:ND2	1:A:305:ASN:O	2.55	0.40
1:A:154:ASN:HA	1:A:181:GLY:C	2.45	0.40
1:A:189:PRO:O	1:A:192:LEU:N	2.50	0.40
2:B:34:LYS:HA	7:B:1167:HOH:O	2.21	0.40
2:B:141:CYS:SG	2:B:143:LYS:HG2	2.61	0.40
2:D:130:ARG:HB2	2:D:133:ASP:O	2.21	0.40
1:A:66:LEU:CD2	1:A:297:GLN:HE21	2.34	0.40
1:C:227:MET:HE3	1:C:227:MET:HB3	1.72	0.40
1:C:292:GLY:O	1:C:296:ARG:HB2	2.20	0.40
1:A:108:GLN:HG3	2:B:113:ASN:O	2.21	0.40
1:A:132:ASN:ND2	2:B:143:LYS:NZ	2.70	0.40
1:C:5:TYR:CZ	1:C:6:GLN:HG2	2.57	0.40
2:D:13:LYS:HG3	2:D:88:ASN:HA	2.04	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	308/310 (99%)	284 (92%)	22 (7%)	2 (1%)	21	18
1	C	308/310 (99%)	286 (93%)	17 (6%)	5 (2%)	7	4
2	B	151/153 (99%)	123 (82%)	21 (14%)	7 (5%)	2	0
2	D	151/153 (99%)	124 (82%)	18 (12%)	9 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	918/926 (99%)	817 (89%)	78 (8%)	23 (2%)	4 1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	HIS
2	B	12	ILE
2	B	106	VAL
2	D	6	LYS
2	D	9	VAL
2	D	24	GLN
2	B	51	GLY
2	B	105	ASN
1	C	41	HIS
2	D	89	TYR
2	D	118	ALA
1	A	85	GLY
1	C	80	SER
1	C	271	ASP
1	C	76	SER
2	D	52	GLU
1	A	75	ASP
2	B	37	GLU
2	B	134	ILE
2	D	7	LEU
2	D	75	ALA
2	D	120	PRO
1	C	270	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	260/260 (100%)	208 (80%)	52 (20%)	1 0
1	C	260/260 (100%)	212 (82%)	48 (18%)	1 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	137/137 (100%)	94 (69%)	43 (31%)	0	0
2	D	137/137 (100%)	96 (70%)	41 (30%)	0	0
All	All	794/794 (100%)	610 (77%)	184 (23%)	1	0

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	17	ARG
1	A	31	LYS
1	A	38	LEU
1	A	40	LYS
1	A	42	LYS
1	A	52	SER
1	A	53	THR
1	A	57	LEU
1	A	78	ASN
1	A	79	THR
1	A	80	SER
1	A	81	LEU
1	A	108	GLN
1	A	116	THR
1	A	121	ASN
1	A	124	VAL
1	A	140	LEU
1	A	146	GLN
1	A	149	GLN
1	A	151	ARG
1	A	160	VAL
1	A	164	LYS
1	A	167	ARG
1	A	169	VAL
1	A	183	ARG
1	A	201	MET
1	A	204	GLU
1	A	205	LYS
1	A	211	LEU
1	A	213	SER
1	A	215	ILE
1	A	227	MET
1	A	229	ARG

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Mol	Chain	Res	Type
1	A	231	GLN
1	A	232	LYS
1	A	233	GLU
1	A	235	LEU
1	A	238	SER
1	A	239	GLU
1	A	248	VAL
1	A	249	LEU
1	A	250	ARG
1	A	252	SER
1	A	258	LYS
1	A	267	LEU
1	A	269	ARG
1	A	279	LYS
1	A	285	TYR
1	A	302	LEU
1	A	309	VAL
1	A	310	LEU
2	B	4	ASP
2	B	5	ASN
2	B	6	LYS
2	B	7	LEU
2	B	9	VAL
2	B	10	GLU
2	B	12	ILE
2	B	21	ILE
2	B	31	SER
2	B	32	LEU
2	B	38	THR
2	B	40	GLN
2	B	41	ARG
2	B	50	SER
2	B	52	GLU
2	B	53	MET
2	B	55	ARG
2	B	56	LYS
2	B	58	LEU
2	B	66	LEU
2	B	68	GLU
2	B	70	GLN
2	B	74	LEU
2	B	76	LEU

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Mol	Chain	Res	Type
2	B	80	GLN
2	B	82	THR
2	B	85	ARG
2	B	86	ILE
2	B	90	GLU
2	B	92	VAL
2	B	95	SER
2	B	98	SER
2	B	99	LEU
2	B	102	ARG
2	B	105	ASN
2	B	106	VAL
2	B	107	LEU
2	B	122	SER
2	B	127	VAL
2	B	130	ARG
2	B	137	LYS
2	B	143	LYS
2	B	149	VAL
1	C	7	LYS
1	C	12	ILE
1	C	17	ARG
1	C	29	LYS
1	C	57	LEU
1	C	66	LEU
1	C	74	SER
1	C	75	ASP
1	C	80	SER
1	C	81	LEU
1	C	83	LYS
1	C	84	LYS
1	C	86	GLU
1	C	96	SER
1	C	108	GLN
1	C	117	GLU
1	C	140	LEU
1	C	147	GLU
1	C	153	ASP
1	C	159	MET
1	C	167	ARG
1	C	171	SER
1	C	174	GLN

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Mol	Chain	Res	Type
1	C	178	LYS
1	C	190	ASP
1	C	201	MET
1	C	210	SER
1	C	215	ILE
1	C	216	GLU
1	C	227	MET
1	C	229	ARG
1	C	239	GLU
1	C	243	VAL
1	C	244	LYS
1	C	246	GLN
1	C	258	LYS
1	C	272	GLU
1	C	279	LYS
1	C	285	TYR
1	C	291	ASN
1	C	299	LEU
1	C	303	VAL
1	C	305	ASN
1	C	306	ARG
1	C	307	ASP
1	C	308	LEU
1	C	309	VAL
1	C	310	LEU
2	D	1	MET
2	D	2	THR
2	D	3	HIS
2	D	8	GLN
2	D	10	GLU
2	D	12	ILE
2	D	18	ILE
2	D	21	ILE
2	D	34	LYS
2	D	40	GLN
2	D	41	ARG
2	D	48	LEU
2	D	53	MET
2	D	55	ARG
2	D	61	ILE
2	D	62	GLU
2	D	64	THR

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Mol	Chain	Res	Type
2	D	69	ASP
2	D	73	GLN
2	D	74	LEU
2	D	76	LEU
2	D	80	GLN
2	D	84	ASN
2	D	85	ARG
2	D	91	VAL
2	D	92	VAL
2	D	95	SER
2	D	98	SER
2	D	101	GLU
2	D	102	ARG
2	D	109	CYS
2	D	124	SER
2	D	128	ARG
2	D	129	LYS
2	D	130	ARG
2	D	134	ILE
2	D	137	LYS
2	D	141	CYS
2	D	143	LYS
2	D	149	VAL
2	D	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	13	ASN
1	A	21	ASN
1	A	132	ASN
1	A	137	GLN
1	A	154	ASN
1	A	156	HIS
1	A	212	HIS
1	A	255	HIS
1	A	291	ASN
1	A	297	GLN
1	A	305	ASN
2	B	3	HIS
2	B	8	GLN

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Mol	Chain	Res	Type
2	B	63	ASN
2	B	73	GLN
2	B	105	ASN
2	B	153	ASN
1	C	6	GLN
1	C	8	HIS
1	C	33	ASN
1	C	137	GLN
1	C	174	GLN
1	C	255	HIS
1	C	288	GLN
1	C	291	ASN
2	D	40	GLN
2	D	63	ASN
2	D	70	GLN
2	D	80	GLN
2	D	84	ASN
2	D	132	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
6	CTP	B	1156	-	29,30,30	2.84	10 (34%)	43,47,47	3.23	15 (34%)
4	PCT	C	1313	-	7,7,7	3.19	4 (57%)	9,10,10	1.50	2 (22%)
3	MLI	A	1312	-	6,6,6	1.02	0	7,7,7	1.20	1 (14%)
4	PCT	A	1314	-	7,7,7	3.13	4 (57%)	9,10,10	1.43	2 (22%)
6	CTP	D	1157	-	29,30,30	2.87	10 (34%)	43,47,47	3.69	16 (37%)
3	MLI	C	1311	-	6,6,6	1.06	0	7,7,7	1.24	1 (14%)

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
6	CTP	B	1156	-	-	6/22/38/38	0/2/2/2
4	PCT	C	1313	-	-	4/4/5/5	-
3	MLI	A	1312	-	-	4/4/4/4	-
4	PCT	A	1314	-	-	1/4/5/5	-
6	CTP	D	1157	-	-	0/22/38/38	0/2/2/2
3	MLI	C	1311	-	-	2/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1157	CTP	PB-O3B	7.53	1.67	1.59
6	D	1157	CTP	C4-N3	7.40	1.49	1.34
6	B	1156	CTP	C4-N3	7.37	1.49	1.34
6	B	1156	CTP	PB-O3B	7.19	1.67	1.59
6	D	1157	CTP	C2-N3	6.76	1.49	1.36
6	B	1156	CTP	C2-N3	6.68	1.49	1.36
4	A	1314	PCT	P-O1P	5.25	1.60	1.50
4	C	1313	PCT	P-O1P	5.00	1.60	1.50
4	C	1313	PCT	P-C1P	4.95	1.87	1.79
4	A	1314	PCT	P-C1P	4.63	1.86	1.79
6	B	1156	CTP	C2-N1	4.41	1.49	1.40
6	D	1157	CTP	C2-N1	4.23	1.48	1.40
6	D	1157	CTP	PB-O3A	3.57	1.63	1.59
6	D	1157	CTP	PG-O1G	3.54	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1156	CTP	PG-O1G	3.48	1.61	1.50
6	B	1156	CTP	PB-O3A	3.44	1.63	1.59
4	C	1313	PCT	P-O3P	3.43	1.62	1.55
4	A	1314	PCT	P-O3P	3.35	1.62	1.55
6	B	1156	CTP	PA-O1A	2.91	1.60	1.50
6	D	1157	CTP	PA-O1A	2.67	1.60	1.50
6	B	1156	CTP	PA-O3A	2.61	1.62	1.59
4	A	1314	PCT	P-O2P	2.50	1.60	1.55
4	C	1313	PCT	P-O2P	2.46	1.60	1.55
6	D	1157	CTP	PB-O1B	2.27	1.58	1.50
6	B	1156	CTP	PG-O3G	2.20	1.63	1.54
6	D	1157	CTP	PG-O3G	2.09	1.62	1.54
6	D	1157	CTP	C6-C5	2.06	1.39	1.35
6	B	1156	CTP	C6-C5	2.01	1.39	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1157	CTP	O2B-PB-O3A	17.67	155.02	107.27
6	B	1156	CTP	O2B-PB-O3A	11.07	137.19	107.27
6	B	1156	CTP	O2G-PG-O3B	8.75	133.99	104.64
6	B	1156	CTP	O3A-PB-O1B	-8.07	86.44	110.70
6	D	1157	CTP	O3G-PG-O3B	-7.59	79.19	104.64
6	B	1156	CTP	C6-N1-C2	-6.46	109.56	120.46
6	D	1157	CTP	O3B-PG-O1G	6.21	143.73	111.04
6	B	1156	CTP	C5-C6-N1	5.63	130.99	121.84
6	D	1157	CTP	C6-N1-C2	-5.17	111.73	120.46
6	D	1157	CTP	O3A-PB-O1B	-5.10	95.38	110.70
6	D	1157	CTP	C5-C6-N1	4.45	129.07	121.84
6	B	1156	CTP	O3B-PG-O1G	-3.92	90.41	111.04
6	D	1157	CTP	O2-C2-N3	-3.70	116.50	122.33
6	B	1156	CTP	O2-C2-N3	-3.64	116.59	122.33
6	B	1156	CTP	C5-C4-N3	-2.95	116.35	121.32
6	B	1156	CTP	C3'-C2'-C1'	2.91	106.97	101.46
6	D	1157	CTP	O2A-PA-O3A	2.79	114.82	107.27
6	D	1157	CTP	C3'-C2'-C1'	2.76	106.69	101.46
3	C	1311	MLI	C3-C1-C2	2.73	122.58	112.95
6	D	1157	CTP	O2G-PG-O1G	-2.69	100.36	110.83
3	A	1312	MLI	C3-C1-C2	2.53	121.88	112.95
6	B	1156	CTP	O2G-PG-O1G	-2.48	101.16	110.83
4	C	1313	PCT	O1-C1-C1P	2.47	122.46	119.86
6	B	1156	CTP	N1-C2-N3	2.46	123.08	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1157	CTP	O4'-C4'-C3'	2.46	110.03	105.15
6	D	1157	CTP	C6-C5-C4	2.41	121.48	117.53
6	D	1157	CTP	C5-C4-N3	-2.40	117.28	121.32
4	A	1314	PCT	O3P-P-O2P	2.38	114.75	107.96
6	B	1156	CTP	C5'-C4'-C3'	-2.38	106.66	115.21
6	D	1157	CTP	O2A-PA-O5'	-2.36	96.87	107.57
6	B	1156	CTP	O2A-PA-O3A	2.36	113.64	107.27
6	B	1156	CTP	C6-C5-C4	2.31	121.31	117.53
4	A	1314	PCT	O1P-P-C1P	-2.27	105.84	111.10
4	C	1313	PCT	O1P-P-C1P	-2.17	106.08	111.10
6	B	1156	CTP	O4'-C1'-C2'	-2.15	102.01	106.62
6	D	1157	CTP	N1-C2-N3	2.06	122.38	118.80
6	D	1157	CTP	O2A-PA-O1A	-2.02	103.05	112.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1314	PCT	O1-C1-C1P-P
4	C	1313	PCT	O1-C1-C1P-P
6	B	1156	CTP	C5'-O5'-PA-O2A
6	B	1156	CTP	C5'-O5'-PA-O3A
6	B	1156	CTP	PB-O3B-PG-O3G
4	C	1313	PCT	C1-C1P-P-O2P
4	C	1313	PCT	C1-C1P-P-O3P
3	A	1312	MLI	C2-C1-C3-O8
3	A	1312	MLI	C2-C1-C3-O9
3	A	1312	MLI	C3-C1-C2-O7
6	B	1156	CTP	C5'-O5'-PA-O1A
3	A	1312	MLI	C3-C1-C2-O6
3	C	1311	MLI	C3-C1-C2-O7
6	B	1156	CTP	PB-O3B-PG-O1G
6	B	1156	CTP	PB-O3B-PG-O2G
3	C	1311	MLI	C3-C1-C2-O6
4	C	1313	PCT	C1-C1P-P-O1P

There are no ring outliers.

5 monomers are involved in 26 short contacts:

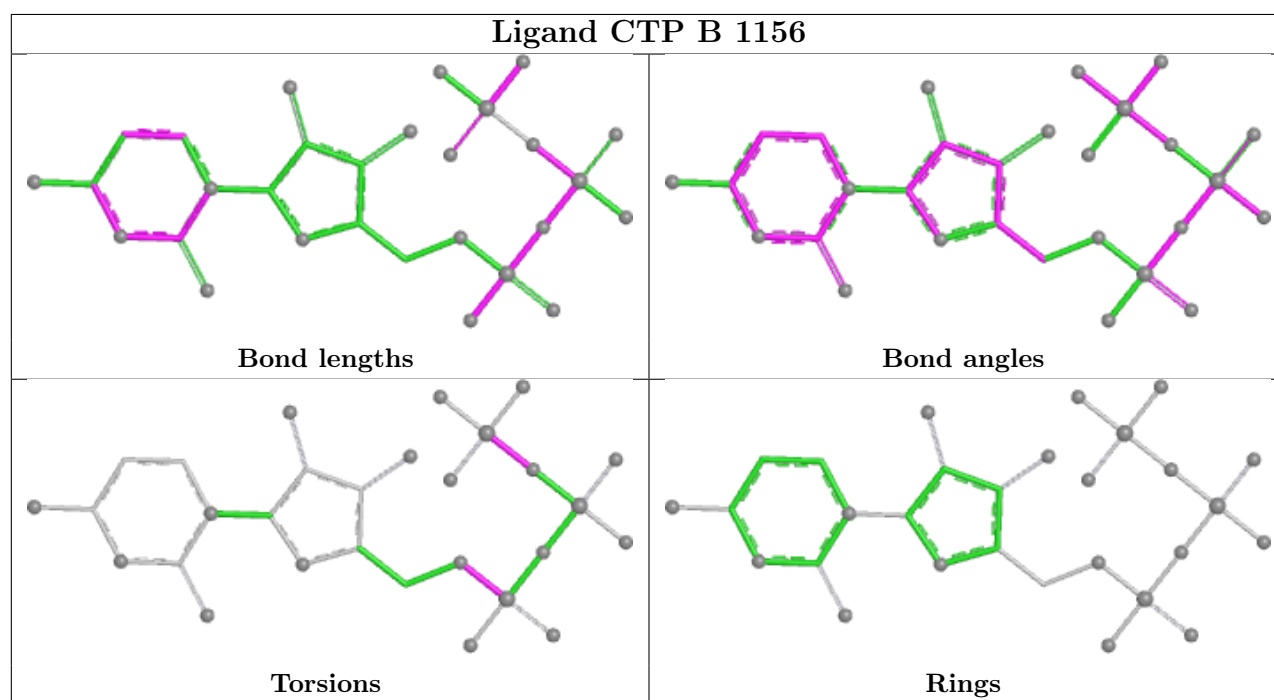
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1156	CTP	7	0

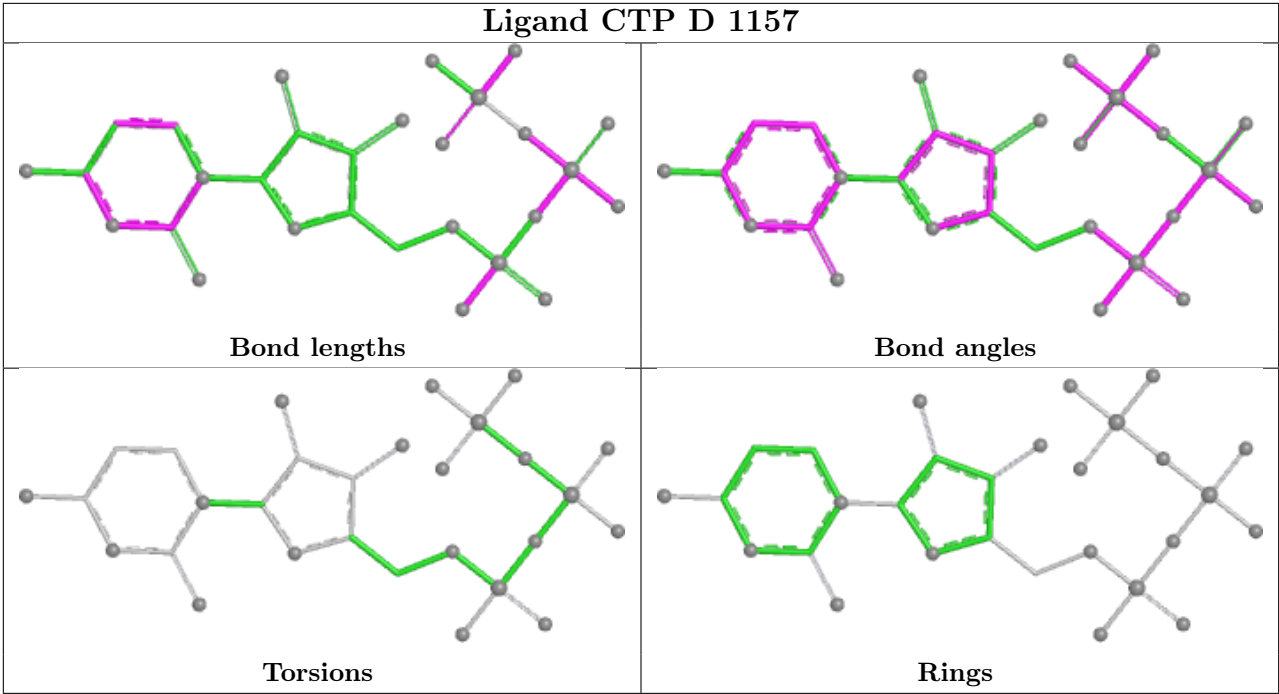
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1313	PCT	5	0
4	A	1314	PCT	3	0
6	D	1157	CTP	7	0
3	C	1311	MLI	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
2	B	3
2	D	2
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	271:ASP	C	272:GLU	N	1.65
1	A	79:THR	C	80:SER	N	1.64
1	A	80:SER	C	81:LEU	N	1.63
1	D	8:GLN	C	9:VAL	N	1.63
1	D	104:ASP	C	105:ASN	N	1.19
1	B	105:ASN	C	106:VAL	N	1.16
1	A	244:LYS	C	245:ALA	N	1.14
1	B	134:ILE	C	135:ALA	N	1.02

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	133:ASP	C	134:ILE	N	0.86

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/310 (100%)	-1.57	0 100 100	7, 25, 95, 158	0
1	C	310/310 (100%)	-1.62	0 100 100	6, 18, 86, 158	0
2	B	153/153 (100%)	-1.35	0 100 100	14, 45, 157, 158	0
2	D	153/153 (100%)	-1.31	0 100 100	13, 47, 156, 158	0
All	All	926/926 (100%)	-1.51	0 100 100	6, 30, 133, 158	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MLI	A	1312	7/7	0.97	0.10	36,56,74,76	7
3	MLI	C	1311	7/7	0.97	0.10	80,81,87,87	7
4	PCT	A	1314	8/8	0.98	0.08	52,72,78,92	8
4	PCT	C	1313	8/8	0.99	0.05	39,53,79,86	8

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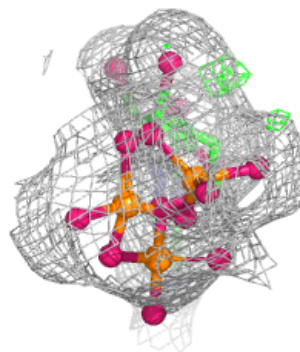
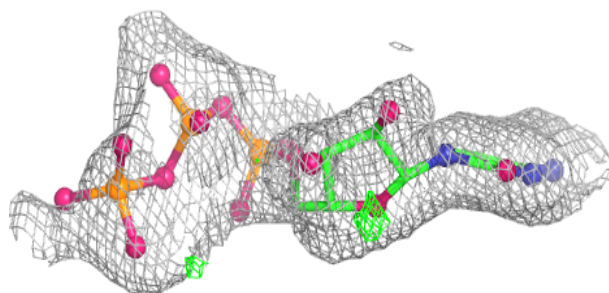
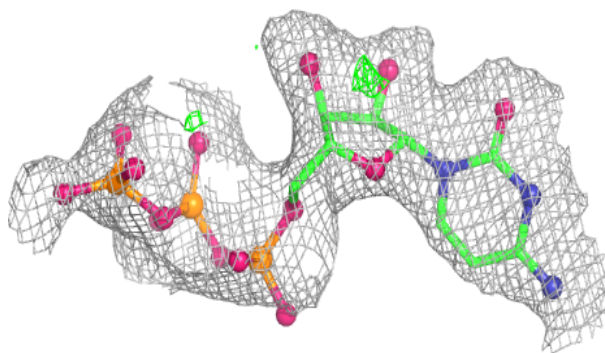
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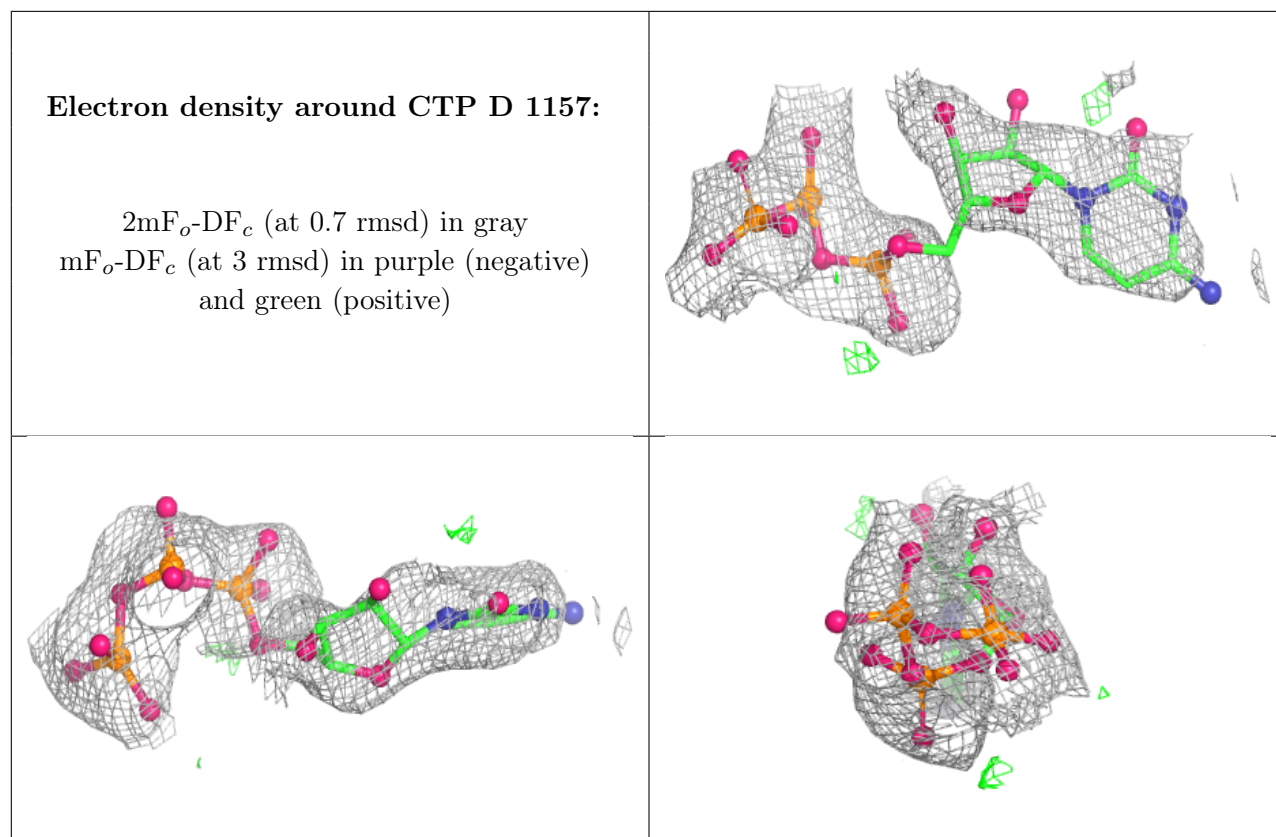
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	D	155	1/1	0.99	0.08	121,121,121,121	1
6	CTP	B	1156	29/29	0.99	0.03	25,40,73,80	0
6	CTP	D	1157	29/29	0.99	0.04	56,79,88,90	29
5	ZN	B	154	1/1	1.00	0.01	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CTP B 1156:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.