



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:46 PM UTC

PDB ID : 1PHH / pdb_00001phh
Title : CRYSTAL STRUCTURE OF P-HYDROXYBENZOATE HYDROXYLASE
COMPLEXED WITH ITS REACTION PRODUCT 3,4-DIHYDROXYBEN
ZOATE
Authors : Schreuder, H.A.; Drenth, J.
Deposited on : 1987-11-04
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

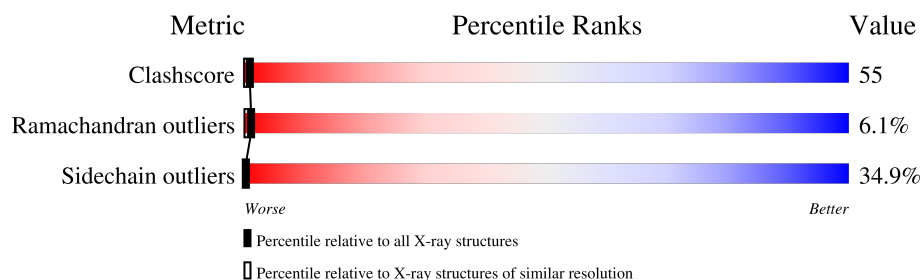
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	16% 37% 31% 16%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3462 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 P-HYDROXYBENZOATE HYDROXYLASE.

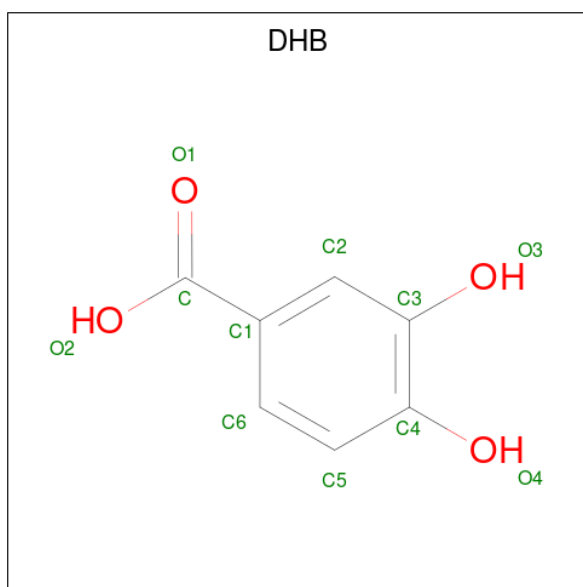
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3125	1976	563	575	11	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is 3,4-DIHYDROXYBENZOIC ACID (CCD ID: DHB) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 4 is water.

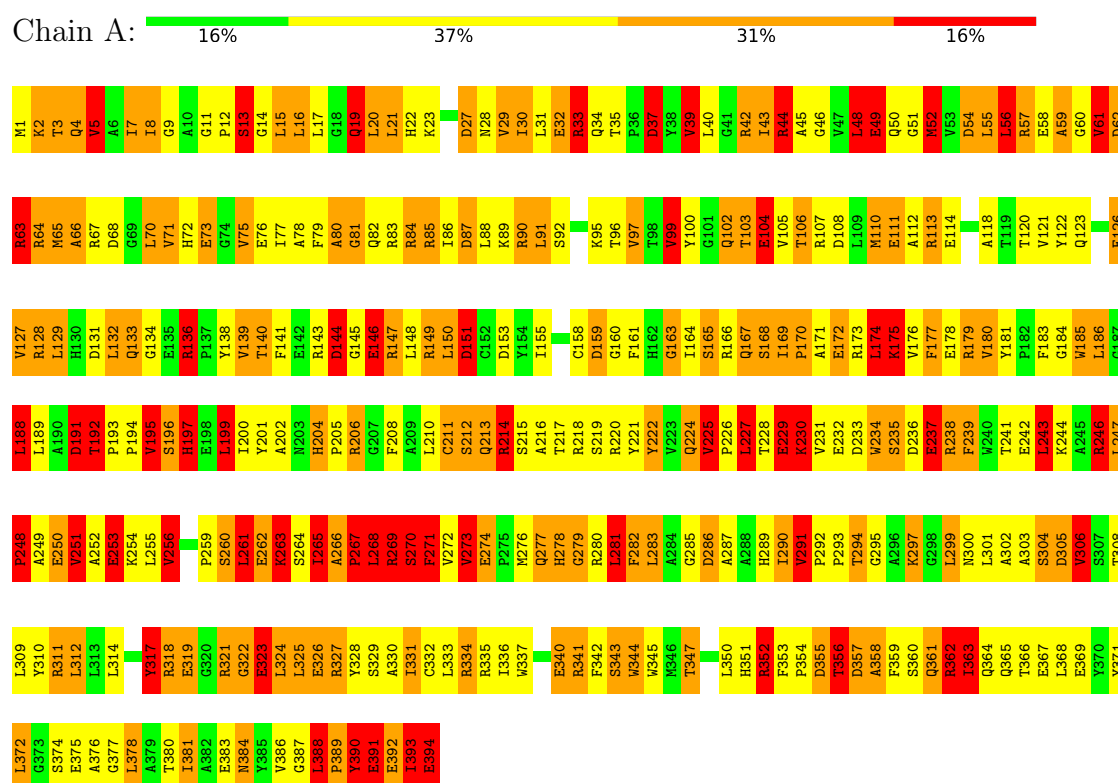
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	273	Total	O	0	0
			273	273		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: P-HYDROXYBENZOATE HYDROXYLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.90Å 146.30Å 88.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3462	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.11	1/3190 (0.0%)	2.85	334/4317 (7.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	LYS	CA-CB	-5.03	1.45	1.53

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ALA	CA-C-N	20.89	145.95	119.84
1	A	266	ALA	C-N-CA	20.89	145.95	119.84
1	A	274	GLU	CA-CB-CG	20.14	154.38	114.10
1	A	175	LYS	CA-CB-CG	18.22	150.54	114.10
1	A	267	PRO	N-CA-C	14.31	141.95	112.47
1	A	111	GLU	CA-CB-CG	14.11	142.31	114.10
1	A	37	ASP	CA-CB-CG	12.68	125.28	112.60
1	A	61	VAL	N-CA-CB	12.56	131.96	111.23
1	A	280	ARG	CD-NE-CZ	12.41	141.77	124.40
1	A	267	PRO	CA-N-CD	-12.32	94.75	112.00
1	A	323	GLU	N-CA-C	-12.28	97.94	113.16
1	A	177	PHE	CA-CB-CG	12.07	125.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	GLN	CB-CG-CD	12.03	133.04	112.60
1	A	243	LEU	N-CA-C	-11.80	98.11	110.97
1	A	196	SER	CA-C-N	11.23	142.99	121.54
1	A	196	SER	C-N-CA	11.23	142.99	121.54
1	A	49	GLU	CB-CG-CD	11.02	131.34	112.60
1	A	236	ASP	N-CA-C	-10.80	98.22	111.40
1	A	248	PRO	N-CA-C	10.67	134.45	112.47
1	A	323	GLU	N-CA-CB	10.34	126.26	110.44
1	A	341	ARG	CA-CB-CG	10.34	134.78	114.10
1	A	324	LEU	N-CA-C	-10.33	99.83	111.71
1	A	214	ARG	CD-NE-CZ	10.32	138.85	124.40
1	A	376	ALA	N-CA-C	-10.23	99.11	111.69
1	A	266	ALA	N-CA-C	10.07	132.07	109.81
1	A	268	LEU	CA-C-O	10.05	132.24	120.99
1	A	375	GLU	CA-CB-CG	10.03	134.15	114.10
1	A	225	VAL	CB-CA-C	10.02	119.15	109.33
1	A	197	HIS	N-CA-C	9.91	131.91	110.80
1	A	326	GLU	N-CA-C	-9.89	101.34	113.41
1	A	52	MET	N-CA-C	-9.85	101.01	113.23
1	A	249	ALA	CA-C-O	9.83	131.75	118.38
1	A	158	CYS	CA-C-O	9.77	132.06	120.53
1	A	180	VAL	CB-CA-C	9.77	125.20	111.81
1	A	229	GLU	N-CA-C	-9.61	95.64	109.96
1	A	200	ILE	N-CA-CB	9.61	124.13	111.64
1	A	68	ASP	N-CA-C	9.45	125.57	112.72
1	A	268	LEU	N-CA-C	9.44	123.80	108.99
1	A	145	GLY	N-CA-C	-9.25	91.26	113.18
1	A	213	GLN	CB-CG-CD	-9.12	97.10	112.60
1	A	66	ALA	N-CA-C	-9.07	101.39	111.28
1	A	357	ASP	N-CA-C	-9.00	96.19	110.14
1	A	32	GLU	CA-C-N	8.98	133.04	120.29
1	A	32	GLU	C-N-CA	8.98	133.04	120.29
1	A	326	GLU	CB-CG-CD	8.96	127.83	112.60
1	A	327	ARG	CD-NE-CZ	8.95	136.93	124.40
1	A	60	GLY	CA-C-N	8.95	138.07	121.97
1	A	60	GLY	C-N-CA	8.95	138.07	121.97
1	A	351	HIS	CA-CB-CG	-8.80	105.00	113.80
1	A	266	ALA	N-CA-CB	-8.71	94.86	110.37
1	A	342	PHE	CA-C-N	8.69	132.63	120.29
1	A	342	PHE	C-N-CA	8.69	132.63	120.29
1	A	191	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	325	LEU	CA-CB-CG	8.57	146.29	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	VAL	O-C-N	8.53	132.47	123.26
1	A	200	ILE	O-C-N	8.52	132.23	123.20
1	A	225	VAL	N-CA-CB	-8.50	102.54	111.64
1	A	212	SER	CA-C-N	8.44	136.99	122.81
1	A	212	SER	C-N-CA	8.44	136.99	122.81
1	A	277	GLN	N-CA-C	8.43	123.21	109.72
1	A	75	VAL	N-CA-CB	8.42	124.31	112.52
1	A	334	ARG	CA-C-O	8.38	129.80	121.00
1	A	276	MET	CA-C-N	8.33	135.88	122.81
1	A	276	MET	C-N-CA	8.33	135.88	122.81
1	A	144	ASP	CA-C-O	8.27	132.33	120.51
1	A	128	ARG	O-C-N	8.22	133.03	123.41
1	A	140	THR	CA-CB-CG2	8.22	124.47	110.50
1	A	60	GLY	N-CA-C	8.13	132.45	113.18
1	A	133	GLN	N-CA-C	-8.11	95.35	108.41
1	A	131	ASP	N-CA-C	8.09	123.10	113.23
1	A	87	ASP	N-CA-CB	8.06	124.12	110.49
1	A	85	ARG	CD-NE-CZ	8.03	135.63	124.40
1	A	192	THR	O-C-N	7.93	130.44	121.32
1	A	144	ASP	CA-C-N	7.89	136.88	121.41
1	A	144	ASP	C-N-CA	7.89	136.88	121.41
1	A	42	ARG	NE-CZ-NH2	-7.87	112.12	119.20
1	A	227	LEU	N-CA-C	7.80	122.52	110.20
1	A	362	ARG	CD-NE-CZ	7.78	135.30	124.40
1	A	261	LEU	N-CA-C	-7.78	94.22	110.80
1	A	188	LEU	CB-CA-C	7.77	121.07	111.43
1	A	153	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	185	TRP	CA-CB-CG	7.74	128.31	113.60
1	A	321	ARG	N-CA-C	7.74	122.14	110.14
1	A	353	PHE	O-C-N	7.72	131.44	121.64
1	A	323	GLU	CA-C-N	7.71	131.38	120.28
1	A	323	GLU	C-N-CA	7.71	131.38	120.28
1	A	324	LEU	CA-CB-CG	7.66	143.10	116.30
1	A	55	LEU	O-C-N	7.65	130.35	122.09
1	A	390	TYR	CA-C-O	-7.59	112.36	120.71
1	A	64	ARG	CA-C-O	-7.56	112.46	120.63
1	A	44	ARG	N-CA-C	7.53	120.05	108.30
1	A	352	ARG	CA-C-O	7.53	130.98	120.52
1	A	146	GLU	CA-CB-CG	7.49	129.09	114.10
1	A	42	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	A	290	ILE	CA-CB-CG2	7.40	123.08	110.50
1	A	384	ASN	CA-CB-CG	7.38	119.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLN	CA-C-O	7.38	129.42	121.16
1	A	56	LEU	N-CA-C	-7.37	103.25	111.28
1	A	299	LEU	N-CA-C	-7.37	102.63	111.69
1	A	111	GLU	CB-CG-CD	7.32	125.04	112.60
1	A	334	ARG	CA-C-N	7.28	130.63	120.29
1	A	334	ARG	C-N-CA	7.28	130.63	120.29
1	A	250	GLU	N-CA-C	-7.26	104.95	113.88
1	A	305	ASP	CB-CA-C	7.24	121.91	109.24
1	A	118	ALA	CA-C-N	7.24	131.11	120.90
1	A	118	ALA	C-N-CA	7.24	131.11	120.90
1	A	343	SER	N-CA-C	7.22	119.22	111.36
1	A	68	ASP	CB-CA-C	-7.20	102.36	111.22
1	A	179	ARG	NE-CZ-NH1	7.20	128.69	121.50
1	A	134	GLY	CA-C-O	-7.14	114.84	121.63
1	A	71	VAL	N-CA-CB	7.14	118.50	110.72
1	A	324	LEU	O-C-N	7.12	130.56	122.22
1	A	63	ARG	CD-NE-CZ	7.12	134.37	124.40
1	A	192	THR	N-CA-CB	7.08	122.96	110.37
1	A	256	VAL	CA-C-O	7.07	127.85	120.36
1	A	29	VAL	N-CA-CB	7.04	121.39	111.82
1	A	99	VAL	N-CA-CB	7.02	120.03	111.60
1	A	147	ARG	N-CA-C	-6.96	98.59	109.25
1	A	230	LYS	N-CA-C	6.96	120.33	110.23
1	A	202	ALA	N-CA-C	6.94	120.97	108.69
1	A	44	ARG	O-C-N	6.92	125.95	120.83
1	A	114	GLU	O-C-N	6.92	129.45	122.12
1	A	269	ARG	N-CA-CB	-6.90	99.98	111.57
1	A	3	THR	CA-C-O	-6.86	114.11	121.45
1	A	62	ASP	N-CA-C	-6.86	101.12	111.34
1	A	179	ARG	CD-NE-CZ	6.82	133.95	124.40
1	A	391	GLU	CB-CA-C	-6.81	96.86	110.42
1	A	251	VAL	CA-C-O	-6.81	112.27	120.78
1	A	20	LEU	N-CA-C	-6.79	104.03	112.72
1	A	253	GLU	N-CA-C	-6.78	104.48	112.89
1	A	118	ALA	CA-C-O	6.76	128.58	120.81
1	A	20	LEU	CA-C-O	6.76	127.72	119.81
1	A	204	HIS	CA-C-O	-6.73	112.26	120.54
1	A	27	ASP	CA-C-N	6.71	133.13	122.59
1	A	27	ASP	C-N-CA	6.71	133.13	122.59
1	A	331	ILE	CA-C-N	6.70	130.50	120.31
1	A	331	ILE	C-N-CA	6.70	130.50	120.31
1	A	251	VAL	N-CA-C	6.70	123.27	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASP	O-C-N	6.68	128.34	121.79
1	A	294	THR	N-CA-C	6.67	125.01	110.80
1	A	58	GLU	CA-CB-CG	6.66	127.41	114.10
1	A	353	PHE	CA-C-O	-6.64	113.80	120.64
1	A	134	GLY	N-CA-C	-6.62	100.55	110.42
1	A	33	ARG	NE-CZ-NH2	-6.62	113.24	119.20
1	A	318	ARG	CA-C-O	-6.62	113.40	120.42
1	A	266	ALA	O-C-N	-6.61	113.72	121.32
1	A	102	GLN	N-CA-C	6.59	119.02	111.11
1	A	222	TYR	O-C-N	6.57	130.74	123.25
1	A	271	PHE	CA-CB-CG	6.54	120.34	113.80
1	A	389	PRO	CB-CA-C	6.53	121.46	111.40
1	A	390	TYR	N-CA-C	6.52	123.20	110.56
1	A	227	LEU	CA-C-O	6.51	128.47	121.05
1	A	290	ILE	CB-CA-C	6.50	120.55	110.28
1	A	377	GLY	CA-C-N	6.49	128.88	120.44
1	A	377	GLY	C-N-CA	6.49	128.88	120.44
1	A	136	ARG	CD-NE-CZ	6.48	133.47	124.40
1	A	159	ASP	O-C-N	6.47	129.79	122.22
1	A	364	GLN	CA-C-N	6.45	129.22	120.44
1	A	364	GLN	C-N-CA	6.45	129.22	120.44
1	A	251	VAL	N-CA-CB	-6.44	100.61	111.23
1	A	319	GLU	CB-CG-CD	6.41	123.49	112.60
1	A	48	LEU	CA-CB-CG	6.40	138.71	116.30
1	A	113	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	291	VAL	N-CA-CB	6.39	120.16	111.21
1	A	37	ASP	N-CA-CB	6.36	121.66	110.27
1	A	265	ILE	N-CA-C	6.35	122.55	109.34
1	A	49	GLU	CA-CB-CG	6.33	126.77	114.10
1	A	383	GLU	CA-C-O	-6.28	113.89	120.92
1	A	199	LEU	CA-C-N	-6.27	114.76	123.10
1	A	199	LEU	C-N-CA	-6.27	114.76	123.10
1	A	341	ARG	CB-CG-CD	6.25	125.68	111.30
1	A	33	ARG	CA-CB-CG	6.24	126.58	114.10
1	A	158	CYS	CA-C-N	6.23	129.25	120.28
1	A	158	CYS	C-N-CA	6.23	129.25	120.28
1	A	82	GLN	N-CA-C	6.22	116.78	108.38
1	A	104	GLU	CA-CB-CG	6.20	126.50	114.10
1	A	234	TRP	CA-CB-CG	-6.19	101.83	113.60
1	A	68	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	243	LEU	CB-CA-C	6.19	120.49	110.96
1	A	327	ARG	CA-CB-CG	6.17	126.44	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	CD-NE-CZ	-6.17	115.76	124.40
1	A	375	GLU	CG-CD-OE1	6.16	132.58	118.40
1	A	183	PHE	CA-C-O	-6.15	114.23	121.06
1	A	49	GLU	CA-C-O	-6.14	114.75	121.87
1	A	183	PHE	O-C-N	6.13	128.93	123.41
1	A	196	SER	N-CA-C	-6.12	97.16	107.99
1	A	269	ARG	N-CA-C	6.12	117.44	108.14
1	A	104	GLU	CB-CA-C	-6.12	100.51	110.79
1	A	212	SER	CA-C-O	6.11	127.99	121.45
1	A	213	GLN	OE1-CD-NE2	6.10	128.70	122.60
1	A	8	ILE	CA-C-O	-6.09	113.33	120.75
1	A	343	SER	CA-CB-OG	-6.08	98.93	111.10
1	A	139	VAL	CA-CB-CG1	6.08	120.74	110.40
1	A	282	PHE	CA-C-O	-6.07	112.79	120.20
1	A	265	ILE	CA-C-N	6.04	136.55	121.80
1	A	265	ILE	C-N-CA	6.04	136.55	121.80
1	A	237	GLU	CA-C-O	-6.04	114.15	120.55
1	A	391	GLU	CA-C-N	6.02	133.05	121.54
1	A	391	GLU	C-N-CA	6.02	133.05	121.54
1	A	113	ARG	N-CA-CB	6.00	119.05	110.16
1	A	260	SER	O-C-N	6.00	130.12	123.16
1	A	86	ILE	CA-C-O	-6.00	114.66	120.30
1	A	5	VAL	CA-C-O	-5.97	114.12	120.39
1	A	196	SER	CB-CA-C	5.97	120.51	110.79
1	A	357	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	388	LEU	CB-CA-C	5.96	125.89	111.89
1	A	110	MET	N-CA-C	-5.95	105.51	112.89
1	A	264	SER	CA-C-O	-5.94	112.74	119.98
1	A	56	LEU	CB-CA-C	5.93	120.64	110.79
1	A	236	ASP	CB-CA-C	5.93	120.75	110.79
1	A	33	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	A	356	THR	CA-C-O	5.91	128.97	120.51
1	A	259	PRO	CB-CA-C	5.91	118.72	110.98
1	A	169	ILE	N-CA-CB	5.90	119.47	111.21
1	A	337	TRP	CA-C-O	-5.90	114.24	120.55
1	A	319	GLU	CB-CA-C	5.89	122.05	111.03
1	A	103	THR	CA-CB-OG1	-5.89	100.76	109.60
1	A	13	SER	CA-C-N	5.87	126.61	120.03
1	A	13	SER	C-N-CA	5.87	126.61	120.03
1	A	357	ASP	CB-CA-C	5.87	120.28	109.71
1	A	238	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	A	39	VAL	CB-CA-C	5.85	120.29	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	CA-C-N	5.82	129.74	121.42
1	A	84	ARG	C-N-CA	5.82	129.74	121.42
1	A	204	HIS	O-C-N	5.81	128.24	121.39
1	A	253	GLU	CA-C-N	5.81	128.34	120.44
1	A	253	GLU	C-N-CA	5.81	128.34	120.44
1	A	364	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	192	THR	N-CA-C	-5.79	97.01	109.81
1	A	311	ARG	N-CA-C	-5.76	105.08	111.36
1	A	278	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	19	GLN	CA-C-O	-5.74	112.31	120.51
1	A	326	GLU	CA-CB-CG	5.73	125.57	114.10
1	A	306	VAL	N-CA-C	-5.72	103.94	111.09
1	A	341	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	A	363	ILE	CA-C-N	5.69	127.91	120.28
1	A	363	ILE	C-N-CA	5.69	127.91	120.28
1	A	327	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	A	263	LYS	CA-C-N	5.67	130.76	121.58
1	A	263	LYS	C-N-CA	5.67	130.76	121.58
1	A	128	ARG	CD-NE-CZ	-5.66	116.48	124.40
1	A	305	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	239	PHE	CA-C-O	5.66	126.74	120.80
1	A	391	GLU	N-CA-C	5.66	122.84	110.80
1	A	261	LEU	O-C-N	5.65	130.10	122.59
1	A	256	VAL	CB-CA-C	5.65	118.58	110.33
1	A	113	ARG	O-C-N	5.65	128.59	122.15
1	A	22	HIS	CA-CB-CG	-5.64	108.16	113.80
1	A	106	THR	CA-C-O	-5.63	113.99	120.24
1	A	63	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	A	326	GLU	N-CA-CB	5.59	118.64	110.47
1	A	388	LEU	N-CA-C	-5.59	100.85	109.41
1	A	155	ILE	CB-CA-C	-5.59	102.80	110.96
1	A	16	LEU	CB-CA-C	5.59	119.81	110.92
1	A	325	LEU	CB-CA-C	5.56	120.68	110.11
1	A	3	THR	O-C-N	5.56	129.49	123.10
1	A	179	ARG	NH1-CZ-NH2	-5.55	112.09	119.30
1	A	318	ARG	N-CA-C	5.55	117.41	111.36
1	A	347	THR	O-C-N	5.54	127.86	122.09
1	A	204	HIS	N-CA-C	-5.52	102.50	110.40
1	A	139	VAL	CA-C-N	5.51	130.55	122.77
1	A	139	VAL	C-N-CA	5.51	130.55	122.77
1	A	340	GLU	CA-C-O	5.48	126.57	120.82
1	A	208	PHE	CA-CB-CG	5.47	119.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	SER	CA-C-O	-5.46	112.88	119.49
1	A	387	GLY	CA-C-N	-5.45	114.22	122.29
1	A	387	GLY	C-N-CA	-5.45	114.22	122.29
1	A	128	ARG	CA-C-O	-5.45	113.84	120.54
1	A	347	THR	CA-C-O	-5.44	115.08	120.90
1	A	197	HIS	CB-CA-C	-5.44	99.59	110.42
1	A	213	GLN	O-C-N	5.43	130.39	123.11
1	A	163	GLY	O-C-N	5.40	129.50	122.91
1	A	321	ARG	N-CA-CB	-5.39	102.54	110.85
1	A	20	LEU	CA-C-N	5.38	127.44	120.44
1	A	20	LEU	C-N-CA	5.38	127.44	120.44
1	A	345	TRP	N-CA-C	-5.38	105.11	110.97
1	A	81	GLY	O-C-N	5.36	129.67	122.70
1	A	86	ILE	CB-CA-C	5.36	116.45	111.30
1	A	85	ARG	O-C-N	5.36	129.34	123.01
1	A	159	ASP	N-CA-C	5.34	117.85	111.71
1	A	195	VAL	CA-C-N	5.34	130.69	123.11
1	A	195	VAL	C-N-CA	5.34	130.69	123.11
1	A	270	SER	CA-C-O	-5.34	114.94	120.70
1	A	97	VAL	CA-CB-CG1	5.32	119.45	110.40
1	A	172	GLU	CB-CG-CD	5.32	121.65	112.60
1	A	199	LEU	CB-CA-C	5.32	118.31	109.53
1	A	375	GLU	CA-C-O	5.29	126.03	119.79
1	A	78	ALA	CA-C-O	-5.28	115.05	121.28
1	A	151	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	304	SER	O-C-N	5.27	129.24	122.39
1	A	196	SER	O-C-N	-5.26	116.50	123.13
1	A	367	GLU	N-CA-CB	5.26	118.44	110.28
1	A	234	TRP	CB-CA-C	5.25	125.19	113.33
1	A	3	THR	N-CA-CB	5.24	119.84	111.56
1	A	340	GLU	CA-CB-CG	5.22	124.55	114.10
1	A	200	ILE	CA-C-O	-5.22	114.96	120.39
1	A	273	VAL	O-C-N	5.22	128.64	122.69
1	A	204	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	172	GLU	N-CA-C	-5.19	106.64	112.87
1	A	383	GLU	CA-CB-CG	5.18	124.47	114.10
1	A	281	LEU	CA-C-O	-5.18	115.05	120.80
1	A	131	ASP	CA-CB-CG	-5.17	107.43	112.60
1	A	86	ILE	N-CA-C	5.17	116.09	111.90
1	A	291	VAL	O-C-N	5.16	126.98	121.10
1	A	73	GLU	O-C-N	5.16	128.79	122.34
1	A	246	ARG	CA-CB-CG	5.16	124.42	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	62	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	323	GLU	CA-C-O	5.15	125.51	119.28
1	A	54	ASP	O-C-N	5.14	128.59	122.27
1	A	211	CYS	CB-CA-C	5.14	118.23	109.80
1	A	11	GLY	N-CA-C	-5.13	101.87	112.34
1	A	186	LEU	CA-C-O	-5.11	115.22	120.54
1	A	249	ALA	N-CA-C	-5.11	106.06	113.21
1	A	229	GLU	CA-C-N	5.11	127.96	120.71
1	A	229	GLU	C-N-CA	5.11	127.96	120.71
1	A	277	GLN	CB-CA-C	-5.10	99.28	109.33
1	A	229	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	256	VAL	CA-CB-CG1	5.10	119.07	110.40
1	A	250	GLU	CA-C-O	5.09	124.99	119.24
1	A	61	VAL	N-CA-C	-5.07	98.79	109.34
1	A	325	LEU	N-CA-C	-5.07	107.06	113.20
1	A	235	SER	CA-C-O	-5.07	115.89	121.31
1	A	73	GLU	CA-C-O	-5.06	113.43	119.35
1	A	174	LEU	O-C-N	5.05	129.87	123.11
1	A	54	ASP	N-CA-C	-5.04	105.98	111.82
1	A	49	GLU	CG-CD-OE1	5.03	129.96	118.40
1	A	29	VAL	CA-C-O	-5.03	115.19	120.27
1	A	123	GLN	CB-CG-CD	5.02	121.14	112.60
1	A	317	TYR	CA-CB-CG	-5.01	104.87	113.90
1	A	260	SER	CA-C-O	-5.01	115.16	120.92
1	A	394	GLU	N-CA-CB	5.01	119.01	110.50
1	A	85	ARG	CA-C-N	-5.00	117.81	122.66
1	A	85	ARG	C-N-CA	-5.00	117.81	122.66

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ARG	Sidechain
1	A	33	ARG	Sidechain

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	3125	0	3122	347	4
2	A	53	0	31	1	0
3	A	11	0	3	1	0
4	A	273	0	0	43	0
All	All	3462	0	3156	347	4

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 55.

All (347) 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:A:322:GLY:HA2	1:A:324:LEU:HD12	1.25	1.19
1:A:266:ALA:HB1	1:A:267:PRO:HD2	1.40	1.02
1:A:195:VAL:HG21	1:A:213:GLN:HE21	1.25	1.01
1:A:268:LEU:HD13	1:A:293:PRO:HD2	1.45	0.96
1:A:56:LEU:HG	1:A:61:VAL:HG12	1.49	0.95
1:A:314:LEU:HD22	1:A:318:ARG:HH11	1.32	0.92
1:A:192:THR:N	1:A:193:PRO:HD2	1.88	0.88
1:A:192:THR:N	1:A:193:PRO:CD	2.33	0.88
1:A:266:ALA:HB1	1:A:267:PRO:CD	2.03	0.88
1:A:332:CYS:O	1:A:336:ILE:HG12	1.74	0.87
1:A:40:LEU:HD13	1:A:110:MET:HE3	1.58	0.84
1:A:39:VAL:HB	1:A:42:ARG:NH2	1.91	0.84
1:A:34:GLN:HA	4:A:486:HOH:O	1.78	0.82
1:A:63:ARG:HH22	1:A:67:ARG:NH1	1.78	0.81
1:A:253:GLU:HA	4:A:530:HOH:O	1.79	0.81
1:A:204:HIS:HD2	1:A:206:ARG:H	1.27	0.79
1:A:355:ASP:HA	4:A:491:HOH:O	1.82	0.79
1:A:192:THR:H	1:A:193:PRO:HD2	1.47	0.78
1:A:55:LEU:HD11	4:A:447:HOH:O	1.82	0.78
1:A:218:ARG:NH2	1:A:261:LEU:HG	1.99	0.78
1:A:17:LEU:HG	1:A:21:LEU:HD22	1.66	0.76
1:A:48:LEU:HD21	1:A:100:TYR:HB3	1.66	0.76
1:A:204:HIS:CD2	1:A:206:ARG:H	2.03	0.76
1:A:147:ARG:HH12	1:A:149:ARG:HB2	1.49	0.76
1:A:195:VAL:HG21	1:A:213:GLN:NE2	1.99	0.75
1:A:159:ASP:HB3	1:A:163:GLY:HA3	1.69	0.75
1:A:192:THR:H	1:A:193:PRO:CD	1.95	0.75
1:A:64:ARG:NH1	1:A:67:ARG:HH21	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:HG11	4:A:650:HOH:O	1.87	0.74
1:A:266:ALA:CB	1:A:267:PRO:HD2	2.09	0.74
1:A:230:LYS:O	1:A:233:ASP:HB2	1.88	0.74
1:A:356:THR:HB	1:A:361:GLN:HG2	1.68	0.74
1:A:218:ARG:HH21	1:A:261:LEU:HG	1.54	0.73
1:A:261:LEU:O	1:A:263:LYS:N	2.21	0.73
1:A:356:THR:CB	1:A:361:GLN:HG2	2.18	0.73
1:A:70:LEU:HD22	1:A:70:LEU:H	1.53	0.72
1:A:108:ASP:HA	1:A:111:GLU:HG2	1.70	0.72
1:A:242:GLU:OE1	1:A:246:ARG:NH1	2.22	0.72
1:A:331:ILE:HG12	1:A:392:GLU:OE2	1.90	0.72
1:A:64:ARG:NH1	1:A:67:ARG:NH2	2.38	0.71
1:A:5:VAL:O	1:A:28:ASN:HA	1.90	0.71
1:A:191:ASP:HB3	1:A:261:LEU:HD23	1.71	0.71
1:A:371:TYR:O	1:A:378:LEU:HD13	1.89	0.71
1:A:30:ILE:HG22	1:A:120:THR:HG23	1.72	0.71
1:A:392:GLU:HG3	1:A:393:ILE:H	1.56	0.71
1:A:194:PRO:HD2	1:A:256:VAL:HG12	1.73	0.71
1:A:99:VAL:HG23	4:A:543:HOH:O	1.91	0.71
1:A:308:THR:HG22	1:A:328:TYR:HD1	1.56	0.70
1:A:194:PRO:HD2	1:A:256:VAL:CG1	2.22	0.70
1:A:33:ARG:HD3	1:A:34:GLN:OE1	1.92	0.70
1:A:235:SER:HB2	1:A:238:ARG:HB2	1.73	0.69
1:A:312:LEU:HD23	1:A:328:TYR:HB2	1.71	0.69
1:A:314:LEU:HD22	1:A:318:ARG:NH1	2.06	0.69
1:A:4:GLN:HG2	1:A:317:TYR:CE1	2.27	0.69
1:A:323:GLU:HA	4:A:635:HOH:O	1.91	0.69
1:A:304:SER:CB	1:A:335:ARG:HE	2.05	0.69
1:A:204:HIS:NE2	4:A:465:HOH:O	2.25	0.68
1:A:4:GLN:HG2	1:A:317:TYR:CZ	2.28	0.68
1:A:252:ALA:HB3	1:A:253:GLU:OE2	1.94	0.68
1:A:144:ASP:HB2	1:A:146:GLU:HG2	1.75	0.68
1:A:144:ASP:HB2	1:A:146:GLU:CG	2.24	0.67
1:A:256:VAL:HB	4:A:516:HOH:O	1.94	0.67
1:A:206:ARG:HD2	4:A:465:HOH:O	1.95	0.67
1:A:247:LEU:HB2	1:A:251:VAL:HB	1.77	0.66
1:A:181:TYR:HE2	1:A:292:PRO:HG3	1.60	0.66
1:A:170:PRO:HB2	1:A:173:ARG:HD3	1.77	0.66
1:A:164:ILE:O	1:A:168:SER:OG	2.12	0.66
1:A:329:SER:O	1:A:333:LEU:HB2	1.94	0.66
1:A:230:LYS:HB2	1:A:233:ASP:OD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:HA	4:A:463:HOH:O	1.95	0.65
1:A:218:ARG:HH21	1:A:261:LEU:CG	2.08	0.65
1:A:52:MET:HE3	1:A:303:ALA:CB	2.26	0.65
1:A:52:MET:HE3	1:A:303:ALA:HB1	1.79	0.65
1:A:181:TYR:CE2	1:A:292:PRO:HG3	2.32	0.65
1:A:211:CYS:HA	1:A:221:TYR:CD1	2.32	0.64
1:A:211:CYS:HA	1:A:221:TYR:HD1	1.62	0.64
1:A:246:ARG:C	1:A:247:LEU:HD23	2.22	0.64
1:A:214:ARG:HB2	4:A:533:HOH:O	1.96	0.64
1:A:311:ARG:HH12	1:A:391:GLU:HG3	1.63	0.63
1:A:70:LEU:HD23	1:A:99:VAL:HG22	1.80	0.63
1:A:73:GLU:HB3	1:A:89:LYS:HG2	1.79	0.63
1:A:8:ILE:HD13	1:A:129:LEU:HD21	1.81	0.63
1:A:319:GLU:HB3	1:A:321:ARG:HH12	1.64	0.63
1:A:371:TYR:HB3	1:A:381:ILE:HD11	1.79	0.63
1:A:218:ARG:HH21	1:A:261:LEU:CD2	2.12	0.62
1:A:356:THR:HG21	4:A:623:HOH:O	1.99	0.62
1:A:166:ARG:HD3	1:A:273:VAL:HG21	1.81	0.62
1:A:72:HIS:O	1:A:96:THR:HB	1.99	0.62
1:A:164:ILE:HD11	4:A:591:HOH:O	2.00	0.61
1:A:39:VAL:O	1:A:42:ARG:HB2	2.01	0.61
1:A:52:MET:HE2	1:A:52:MET:O	2.01	0.61
1:A:363:ILE:HG22	4:A:421:HOH:O	2.00	0.60
1:A:175:LYS:HD3	1:A:274:GLU:HG2	1.83	0.60
1:A:128:ARG:C	1:A:129:LEU:HD23	2.26	0.60
1:A:311:ARG:NH1	1:A:391:GLU:OE2	2.35	0.60
1:A:392:GLU:CG	1:A:393:ILE:H	2.13	0.60
1:A:75:VAL:HG12	1:A:199:LEU:HB2	1.84	0.59
1:A:308:THR:CG2	1:A:312:LEU:HD22	2.32	0.59
1:A:67:ARG:HD3	4:A:404:HOH:O	2.02	0.59
1:A:165:SER:HB3	1:A:281:LEU:HD21	1.83	0.59
1:A:174:LEU:HD12	1:A:273:VAL:HB	1.85	0.59
1:A:390:TYR:HB3	1:A:391:GLU:HG2	1.83	0.59
1:A:8:ILE:HG22	1:A:159:ASP:OD1	2.02	0.59
1:A:289:HIS:C	1:A:290:ILE:HG12	2.28	0.59
1:A:144:ASP:HB2	1:A:146:GLU:CB	2.33	0.59
1:A:64:ARG:HH11	1:A:67:ARG:HH21	1.46	0.58
1:A:186:LEU:O	1:A:222:TYR:HA	2.02	0.58
1:A:368:LEU:O	1:A:372:LEU:HB2	2.03	0.58
1:A:57:ARG:HD3	1:A:62:ASP:OD2	2.03	0.58
1:A:271:PHE:HB3	1:A:290:ILE:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLY:O	1:A:99:VAL:HA	2.03	0.58
1:A:57:ARG:NH1	1:A:66:ALA:HB2	2.19	0.58
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.67	0.58
1:A:7:ILE:HB	1:A:30:ILE:HG13	1.85	0.58
1:A:308:THR:HG23	1:A:312:LEU:HD22	1.86	0.58
1:A:322:GLY:CA	1:A:324:LEU:HD12	2.17	0.58
1:A:184:GLY:HA3	1:A:267:PRO:HD3	1.85	0.57
1:A:227:LEU:C	1:A:229:GLU:H	2.11	0.57
1:A:356:THR:OG1	1:A:361:GLN:HG2	2.04	0.57
1:A:173:ARG:NH2	4:A:456:HOH:O	2.37	0.57
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.18	0.57
1:A:295:GLY:O	1:A:297:LYS:HD2	2.04	0.57
1:A:354:PRO:O	1:A:355:ASP:HB2	2.04	0.57
1:A:63:ARG:HH22	1:A:67:ARG:HH12	1.52	0.57
1:A:129:LEU:HD23	1:A:129:LEU:N	2.20	0.56
1:A:161:PHE:HA	1:A:286:ASP:O	2.04	0.56
1:A:161:PHE:CD1	1:A:290:ILE:HG13	2.40	0.56
1:A:87:ASP:O	1:A:91:LEU:HB2	2.05	0.56
1:A:215:SER:OG	1:A:216:ALA:N	2.38	0.56
1:A:107:ARG:HD3	4:A:455:HOH:O	2.06	0.56
1:A:77:ILE:HD13	1:A:201:TYR:HB2	1.86	0.56
1:A:186:LEU:HD11	1:A:231:VAL:HG23	1.87	0.56
1:A:244:LYS:O	1:A:251:VAL:HG21	2.06	0.56
1:A:336:ILE:HG13	4:A:548:HOH:O	2.05	0.56
1:A:108:ASP:HA	1:A:111:GLU:CG	2.36	0.56
1:A:2:LYS:HE3	4:A:513:HOH:O	2.05	0.56
1:A:378:LEU:HA	1:A:381:ILE:HG13	1.88	0.56
1:A:57:ARG:NE	1:A:62:ASP:OD2	2.40	0.55
1:A:146:GLU:O	1:A:148:LEU:HG	2.07	0.55
1:A:237:GLU:HG2	4:A:632:HOH:O	2.06	0.55
1:A:372:LEU:HA	1:A:378:LEU:CD1	2.36	0.55
1:A:220:ARG:HB2	4:A:533:HOH:O	2.04	0.55
1:A:322:GLY:O	1:A:325:LEU:HB3	2.07	0.55
1:A:17:LEU:HG	1:A:21:LEU:CD2	2.37	0.55
1:A:191:ASP:OD1	1:A:191:ASP:O	2.23	0.55
1:A:166:ARG:NE	1:A:287:ALA:O	2.24	0.55
1:A:231:VAL:C	1:A:233:ASP:H	2.14	0.54
1:A:188:LEU:HG	1:A:239:PHE:CD2	2.42	0.54
1:A:262:GLU:HA	1:A:262:GLU:OE1	2.07	0.54
1:A:7:ILE:CG2	1:A:30:ILE:HG13	2.37	0.54
1:A:54:ASP:HA	1:A:57:ARG:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD11	1:A:107:ARG:HB2	1.90	0.54
1:A:144:ASP:HB2	1:A:146:GLU:HB3	1.90	0.53
1:A:17:LEU:O	1:A:21:LEU:HB2	2.07	0.53
1:A:268:LEU:HD12	1:A:292:PRO:HB3	1.90	0.53
1:A:282:PHE:HA	4:A:416:HOH:O	2.08	0.53
1:A:357:ASP:C	1:A:359:PHE:H	2.15	0.53
1:A:49:GLU:OE1	1:A:297:LYS:HE3	2.08	0.53
1:A:294:THR:CG2	1:A:347:THR:OG1	2.57	0.53
1:A:323:GLU:C	1:A:325:LEU:N	2.65	0.53
1:A:374:SER:O	1:A:378:LEU:HD22	2.09	0.53
1:A:271:PHE:CD1	1:A:271:PHE:C	2.87	0.53
1:A:319:GLU:HB3	1:A:321:ARG:NH1	2.23	0.53
1:A:128:ARG:NE	4:A:608:HOH:O	2.42	0.52
1:A:390:TYR:O	1:A:391:GLU:HB3	2.09	0.52
1:A:334:ARG:HD2	4:A:595:HOH:O	2.10	0.52
1:A:234:TRP:CE3	1:A:238:ARG:HD2	2.43	0.52
1:A:48:LEU:CD2	1:A:100:TYR:HB3	2.36	0.52
1:A:164:ILE:O	1:A:164:ILE:HG13	2.08	0.52
1:A:251:VAL:CG2	1:A:251:VAL:O	2.57	0.52
1:A:246:ARG:O	1:A:247:LEU:HD23	2.09	0.52
1:A:45:ALA:HB3	1:A:102:GLN:HB2	1.90	0.52
1:A:314:LEU:HD13	1:A:318:ARG:HH12	1.75	0.52
1:A:330:ALA:O	1:A:334:ARG:HG3	2.10	0.52
1:A:31:LEU:HD21	1:A:141:PHE:CD2	2.45	0.52
1:A:49:GLU:HG2	1:A:300:ASN:CG	2.34	0.52
1:A:128:ARG:HG3	4:A:399:HOH:O	2.10	0.51
1:A:243:LEU:O	1:A:244:LYS:C	2.52	0.51
1:A:393:ILE:O	1:A:394:GLU:HB2	2.10	0.51
1:A:327:ARG:O	1:A:331:ILE:HG13	2.11	0.51
1:A:231:VAL:C	1:A:233:ASP:N	2.68	0.51
1:A:285:GLY:C	1:A:287:ALA:H	2.16	0.51
1:A:285:GLY:O	1:A:287:ALA:N	2.44	0.51
1:A:334:ARG:HB3	4:A:511:HOH:O	2.11	0.51
1:A:244:LYS:HA	1:A:251:VAL:HG23	1.92	0.51
1:A:366:THR:HA	1:A:369:GLU:HG3	1.92	0.51
1:A:368:LEU:O	1:A:372:LEU:HD23	2.10	0.51
1:A:355:ASP:O	1:A:356:THR:C	2.54	0.51
1:A:44:ARG:NH2	4:A:661:HOH:O	2.34	0.51
1:A:56:LEU:HG	1:A:61:VAL:CG1	2.32	0.51
1:A:372:LEU:HA	1:A:378:LEU:HD13	1.93	0.51
1:A:89:LYS:HD2	4:A:657:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HG3	1:A:352:ARG:O	2.10	0.50
1:A:21:LEU:CD1	1:A:310:TYR:HD1	2.24	0.50
1:A:195:VAL:HG13	1:A:219:SER:OG	2.11	0.50
1:A:308:THR:O	1:A:312:LEU:HB2	2.10	0.50
1:A:283:LEU:O	1:A:328:TYR:OH	2.28	0.50
1:A:212:SER:N	1:A:220:ARG:O	2.44	0.50
1:A:214:ARG:HA	1:A:214:ARG:HE	1.76	0.50
1:A:229:GLU:OE2	1:A:234:TRP:NE1	2.35	0.50
1:A:161:PHE:O	1:A:166:ARG:NH2	2.45	0.50
1:A:9:GLY:O	1:A:14:GLY:HA3	2.12	0.49
1:A:108:ASP:O	1:A:111:GLU:HB2	2.11	0.49
1:A:277:GLN:HG2	4:A:416:HOH:O	2.12	0.49
1:A:97:VAL:HG21	4:A:472:HOH:O	2.11	0.49
1:A:304:SER:HB2	1:A:335:ARG:HE	1.75	0.49
1:A:169:ILE:HG23	1:A:278:HIS:CG	2.48	0.49
1:A:189:LEU:HD11	1:A:218:ARG:NE	2.26	0.49
1:A:169:ILE:HD11	1:A:281:LEU:HD13	1.95	0.49
1:A:220:ARG:HH22	1:A:263:LYS:HE2	1.78	0.49
1:A:204:HIS:CD2	1:A:205:PRO:HD2	2.48	0.49
1:A:4:GLN:HB2	1:A:27:ASP:O	2.13	0.48
1:A:81:GLY:HA3	4:A:546:HOH:O	2.13	0.48
1:A:126:GLU:O	1:A:127:VAL:C	2.56	0.48
1:A:16:LEU:HD22	1:A:52:MET:HE1	1.96	0.48
1:A:57:ARG:CD	1:A:62:ASP:OD2	2.61	0.48
1:A:294:THR:HG21	1:A:347:THR:HA	1.95	0.48
1:A:51:GLY:O	1:A:55:LEU:HB2	2.14	0.48
1:A:100:TYR:CZ	1:A:104:GLU:HB3	2.49	0.48
1:A:143:ARG:C	1:A:146:GLU:HG2	2.38	0.48
1:A:79:PHE:O	1:A:80:ALA:C	2.58	0.47
1:A:214:ARG:HE	1:A:214:ARG:CA	2.27	0.47
1:A:70:LEU:H	1:A:70:LEU:CD2	2.23	0.47
1:A:188:LEU:HD22	1:A:260:SER:HB3	1.96	0.47
1:A:191:ASP:CA	1:A:193:PRO:HD2	2.43	0.47
1:A:213:GLN:HG3	1:A:215:SER:O	2.14	0.47
1:A:39:VAL:HB	1:A:42:ARG:HH21	1.71	0.47
1:A:356:THR:HB	1:A:361:GLN:CG	2.40	0.47
1:A:12:PRO:CG	1:A:299:LEU:HD11	2.45	0.47
1:A:243:LEU:HD22	1:A:247:LEU:HD21	1.96	0.47
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.67	0.47
1:A:90:ARG:NH2	4:A:411:HOH:O	2.46	0.47
1:A:185:TRP:O	1:A:266:ALA:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:O	1:A:362:ARG:HB2	2.15	0.47
1:A:43:ILE:HB	1:A:263:LYS:HD2	1.96	0.47
1:A:304:SER:HB3	1:A:335:ARG:HH21	1.79	0.47
1:A:31:LEU:HD12	1:A:121:VAL:HB	1.96	0.47
1:A:238:ARG:HG3	1:A:238:ARG:HH11	1.80	0.47
1:A:52:MET:HE3	1:A:303:ALA:HB2	1.97	0.46
1:A:144:ASP:N	1:A:146:GLU:HG2	2.31	0.46
1:A:238:ARG:HA	1:A:241:THR:HG22	1.97	0.46
1:A:191:ASP:HB3	1:A:218:ARG:NE	2.30	0.46
1:A:278:HIS:O	1:A:279:GLY:C	2.56	0.46
1:A:3:THR:OG1	1:A:4:GLN:N	2.49	0.46
1:A:147:ARG:NH2	4:A:518:HOH:O	2.41	0.46
1:A:149:ARG:NE	4:A:518:HOH:O	2.36	0.46
1:A:160:GLY:HA2	1:A:286:ASP:HB2	1.98	0.46
1:A:265:ILE:HB	1:A:266:ALA:H	1.52	0.46
1:A:362:ARG:HD3	1:A:362:ARG:HA	1.64	0.46
1:A:30:ILE:CG2	1:A:120:THR:HG23	2.44	0.46
1:A:235:SER:HB2	1:A:238:ARG:CB	2.45	0.46
1:A:63:ARG:HG2	4:A:619:HOH:O	2.16	0.45
1:A:33:ARG:NH1	1:A:34:GLN:OE1	2.48	0.45
1:A:356:THR:HG22	1:A:360:SER:OG	2.16	0.45
1:A:57:ARG:C	1:A:59:ALA:H	2.25	0.45
1:A:111:GLU:HB2	1:A:112:ALA:H	1.64	0.45
1:A:224:GLN:HG2	1:A:225:VAL:N	2.29	0.45
1:A:285:GLY:C	1:A:287:ALA:N	2.75	0.45
1:A:84:ARG:NH1	4:A:527:HOH:O	2.48	0.45
1:A:251:VAL:O	1:A:251:VAL:HG22	2.16	0.45
1:A:291:VAL:HG13	1:A:340:GLU:OE2	2.17	0.45
1:A:328:TYR:C	1:A:330:ALA:H	2.25	0.45
1:A:328:TYR:C	1:A:330:ALA:N	2.75	0.45
1:A:191:ASP:HB3	1:A:261:LEU:CD2	2.44	0.45
1:A:322:GLY:C	1:A:324:LEU:N	2.72	0.45
1:A:37:ASP:O	1:A:40:LEU:N	2.50	0.45
1:A:384:ASN:HA	1:A:388:LEU:HD13	1.98	0.45
1:A:144:ASP:CB	1:A:146:GLU:H	2.29	0.44
1:A:357:ASP:O	1:A:359:PHE:N	2.51	0.44
1:A:49:GLU:HB3	1:A:386:VAL:O	2.17	0.44
1:A:301:LEU:HG	1:A:336:ILE:HD12	2.00	0.44
1:A:363:ILE:HD13	1:A:363:ILE:HA	1.69	0.44
1:A:181:TYR:OH	1:A:344:TRP:HB2	2.18	0.44
1:A:19:GLN:NE2	1:A:19:GLN:CA	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:HB2	1:A:303:ALA:CB	2.48	0.44
1:A:174:LEU:CD1	1:A:273:VAL:HB	2.47	0.44
1:A:88:LEU:O	1:A:92:SER:OG	2.20	0.44
1:A:191:ASP:CB	1:A:218:ARG:NE	2.81	0.44
1:A:191:ASP:C	1:A:193:PRO:HD2	2.41	0.44
1:A:49:GLU:CB	1:A:386:VAL:O	2.65	0.43
1:A:106:THR:O	1:A:110:MET:HG3	2.18	0.43
1:A:57:ARG:NH1	1:A:62:ASP:HB3	2.34	0.43
1:A:211:CYS:HB3	1:A:221:TYR:HE1	1.82	0.43
1:A:170:PRO:O	1:A:173:ARG:N	2.41	0.43
1:A:13:SER:OG	1:A:302:ALA:HB1	2.19	0.43
1:A:189:LEU:N	1:A:220:ARG:HH11	2.16	0.43
1:A:392:GLU:HG3	1:A:393:ILE:N	2.30	0.43
1:A:175:LYS:HD3	1:A:274:GLU:CG	2.48	0.43
1:A:220:ARG:HD2	1:A:220:ARG:HA	1.89	0.43
1:A:227:LEU:C	1:A:229:GLU:N	2.77	0.43
1:A:380:THR:O	1:A:384:ASN:ND2	2.45	0.43
1:A:15:LEU:O	1:A:19:GLN:HB2	2.19	0.43
1:A:253:GLU:H	1:A:253:GLU:CD	2.23	0.43
1:A:16:LEU:HD13	1:A:56:LEU:HD12	2.00	0.42
1:A:17:LEU:HD11	1:A:309:LEU:HG	2.01	0.42
1:A:302:ALA:O	1:A:306:VAL:HB	2.19	0.42
1:A:312:LEU:CD2	1:A:328:TYR:HB2	2.44	0.42
1:A:17:LEU:O	1:A:21:LEU:HD22	2.20	0.42
1:A:269:ARG:HG2	1:A:270:SER:N	2.34	0.42
1:A:7:ILE:HG21	1:A:30:ILE:HG13	2.01	0.42
1:A:204:HIS:HD2	1:A:206:ARG:HB2	1.84	0.42
1:A:244:LYS:HD3	1:A:251:VAL:O	2.19	0.42
1:A:293:PRO:O	3:A:396:DHB:O3	2.37	0.42
1:A:309:LEU:O	1:A:309:LEU:HD12	2.18	0.42
1:A:324:LEU:O	1:A:327:ARG:HG2	2.19	0.42
1:A:136:ARG:HB3	4:A:495:HOH:O	2.19	0.42
1:A:204:HIS:HD2	1:A:206:ARG:N	2.06	0.42
1:A:299:LEU:HD12	1:A:299:LEU:HA	1.86	0.42
1:A:57:ARG:HG3	4:A:494:HOH:O	2.18	0.42
1:A:71:VAL:HB	4:A:562:HOH:O	2.20	0.42
1:A:113:ARG:HH11	1:A:113:ARG:HG3	1.84	0.42
1:A:357:ASP:C	1:A:359:PHE:N	2.74	0.42
1:A:389:PRO:HD3	4:A:481:HOH:O	2.19	0.42
1:A:186:LEU:HA	1:A:265:ILE:O	2.20	0.42
1:A:233:ASP:O	1:A:238:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:HH21	1:A:261:LEU:HD23	1.83	0.42
1:A:261:LEU:HA	1:A:261:LEU:HD13	1.61	0.42
1:A:171:ALA:C	1:A:173:ARG:N	2.78	0.42
1:A:247:LEU:HA	1:A:248:PRO:HD3	1.80	0.42
1:A:191:ASP:OD1	1:A:191:ASP:C	2.62	0.42
1:A:225:VAL:HA	1:A:226:PRO:HD3	1.90	0.41
1:A:214:ARG:CZ	4:A:533:HOH:O	2.69	0.41
1:A:28:ASN:OD1	1:A:113:ARG:NH2	2.49	0.41
1:A:77:ILE:HD13	1:A:201:TYR:CB	2.49	0.41
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.81	0.41
1:A:32:GLU:HG2	1:A:122:TYR:CE1	2.55	0.41
1:A:175:LYS:N	1:A:274:GLU:O	2.53	0.41
1:A:128:ARG:HH11	1:A:128:ARG:HD2	1.56	0.41
1:A:133:GLN:NE2	1:A:278:HIS:CE1	2.88	0.41
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.90	0.41
1:A:76:GLU:OE1	1:A:83:ARG:HB3	2.21	0.41
1:A:79:PHE:O	1:A:79:PHE:CD1	2.74	0.41
1:A:84:ARG:NH1	1:A:84:ARG:HG3	2.36	0.41
1:A:149:ARG:NH1	1:A:151:ASP:OD1	2.44	0.41
1:A:210:LEU:O	1:A:221:TYR:HA	2.21	0.41
1:A:289:HIS:O	1:A:290:ILE:HG12	2.20	0.41
1:A:42:ARG:NH2	2:A:395:FAD:O3B	2.54	0.41
1:A:141:PHE:CD2	1:A:141:PHE:N	2.89	0.41
1:A:111:GLU:HA	4:A:615:HOH:O	2.21	0.40
1:A:204:HIS:CD2	1:A:206:ARG:HB2	2.55	0.40
1:A:359:PHE:O	1:A:363:ILE:N	2.48	0.40
1:A:1:MET:HB2	1:A:150:LEU:HD12	2.03	0.40
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.93	0.40
1:A:251:VAL:H	1:A:251:VAL:HG12	1.43	0.40
1:A:343:SER:O	1:A:347:THR:OG1	2.30	0.40
1:A:263:LYS:HE2	1:A:265:ILE:CG1	2.51	0.40
1:A:61:VAL:HG13	1:A:65:MET:HE2	2.03	0.40

All (4) 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)
1:A:1:MET:CE	1:A:192:THR:O[6_565]	1.96	0.24
1:A:23:LYS:O	1:A:57:ARG:NH2[3_556]	2.01	0.19
1:A:138:TYR:OH	1:A:228:THR:OG1[3_656]	2.08	0.12
1:A:1:MET:SD	1:A:192:THR:O[6_565]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	392/394 (100%)	309 (79%)	59 (15%)	24 (6%)	1 0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	146	GLU
1	A	192	THR
1	A	197	HIS
1	A	262	GLU
1	A	267	PRO
1	A	392	GLU
1	A	393	ILE
1	A	59	ALA
1	A	63	ARG
1	A	80	ALA
1	A	265	ILE
1	A	286	ASP
1	A	355	ASP
1	A	356	THR
1	A	358	ALA
1	A	170	PRO
1	A	248	PRO
1	A	391	GLU
1	A	144	ASP
1	A	19	GLN
1	A	317	TYR
1	A	279	GLY
1	A	322	GLY

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	324/324 (100%)	211 (65%)	113 (35%)	0 0

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	4	GLN
1	A	5	VAL
1	A	7	ILE
1	A	13	SER
1	A	15	LEU
1	A	19	GLN
1	A	20	LEU
1	A	21	LEU
1	A	29	VAL
1	A	30	ILE
1	A	35	THR
1	A	37	ASP
1	A	39	VAL
1	A	43	ILE
1	A	44	ARG
1	A	48	LEU
1	A	49	GLU
1	A	50	GLN
1	A	52	MET
1	A	56	LEU
1	A	57	ARG
1	A	63	ARG
1	A	65	MET
1	A	70	LEU
1	A	85	ARG
1	A	90	ARG
1	A	91	LEU
1	A	95	LYS
1	A	99	VAL

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Mol	Chain	Res	Type
1	A	103	THR
1	A	104	GLU
1	A	105	VAL
1	A	126	GLU
1	A	127	VAL
1	A	129	LEU
1	A	132	LEU
1	A	136	ARG
1	A	139	VAL
1	A	140	THR
1	A	144	ASP
1	A	149	ARG
1	A	150	LEU
1	A	151	ASP
1	A	165	SER
1	A	167	GLN
1	A	168	SER
1	A	172	GLU
1	A	174	LEU
1	A	175	LYS
1	A	176	VAL
1	A	177	PHE
1	A	178	GLU
1	A	179	ARG
1	A	180	VAL
1	A	188	LEU
1	A	191	ASP
1	A	192	THR
1	A	195	VAL
1	A	196	SER
1	A	197	HIS
1	A	199	LEU
1	A	214	ARG
1	A	217	THR
1	A	225	VAL
1	A	227	LEU
1	A	229	GLU
1	A	230	LYS
1	A	232	GLU
1	A	237	GLU
1	A	243	LEU
1	A	246	ARG

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Mol	Chain	Res	Type
1	A	247	LEU
1	A	250	GLU
1	A	251	VAL
1	A	253	GLU
1	A	254	LYS
1	A	255	LEU
1	A	256	VAL
1	A	261	LEU
1	A	263	LYS
1	A	265	ILE
1	A	267	PRO
1	A	268	LEU
1	A	269	ARG
1	A	270	SER
1	A	271	PHE
1	A	272	VAL
1	A	273	VAL
1	A	281	LEU
1	A	283	LEU
1	A	291	VAL
1	A	297	LYS
1	A	305	ASP
1	A	306	VAL
1	A	312	LEU
1	A	323	GLU
1	A	326	GLU
1	A	341	ARG
1	A	344	TRP
1	A	350	LEU
1	A	352	ARG
1	A	361	GLN
1	A	362	ARG
1	A	363	ILE
1	A	365	GLN
1	A	372	LEU
1	A	378	LEU
1	A	381	ILE
1	A	388	LEU
1	A	390	TYR
1	A	393	ILE
1	A	394	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	102	GLN
1	A	123	GLN
1	A	197	HIS
1	A	213	GLN
1	A	277	GLN
1	A	365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	FAD	A	395	-	58,58,58	1.75	11 (18%)	85,89,89	1.60	18 (21%)
3	DHB	A	396	-	11,11,11	1.41	2 (18%)	15,15,15	1.39	2 (13%)

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
2	FAD	A	395	-	-	12/34/50/50	0/6/6/6
3	DHB	A	396	-	-	0/4/4/4	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	PA-O3P	-6.18	1.52	1.59
2	A	395	FAD	C9-C8	-4.40	1.33	1.39
2	A	395	FAD	C5'-C4'	3.65	1.56	1.51
3	A	396	DHB	O1-C	3.46	1.32	1.22
2	A	395	FAD	C2A-N1A	3.39	1.40	1.33
2	A	395	FAD	C5A-C4A	3.19	1.44	1.39
2	A	395	FAD	P-O3P	2.83	1.62	1.59
3	A	396	DHB	O2-C	-2.61	1.22	1.30
2	A	395	FAD	P-O2P	-2.54	1.43	1.55
2	A	395	FAD	C6-C7	-2.52	1.36	1.39
2	A	395	FAD	C10-N1	2.16	1.37	1.33
2	A	395	FAD	C4'-C3'	-2.04	1.49	1.53
2	A	395	FAD	O2-C2	-2.00	1.20	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	C9-C9A-N10	4.26	127.58	121.85
2	A	395	FAD	O3P-P-O1P	-3.51	100.15	110.70
2	A	395	FAD	C4A-N9A-C8A	3.33	109.24	105.74
3	A	396	DHB	O2-C-C1	3.16	122.95	114.84
2	A	395	FAD	C10-N1-C2	3.15	123.68	116.85
2	A	395	FAD	C1'-C2'-C3'	3.07	117.99	109.66
2	A	395	FAD	O2P-P-O5'	3.02	121.26	107.57
2	A	395	FAD	C9-C9A-C5X	-2.76	115.16	120.03
2	A	395	FAD	N3A-C2A-N1A	-2.71	124.47	128.58
2	A	395	FAD	C4X-C10-N1	-2.68	118.02	124.59
3	A	396	DHB	O2-C-O1	-2.63	117.69	123.35
2	A	395	FAD	C6-C5X-C9A	2.49	122.46	119.05
2	A	395	FAD	O2P-P-O3P	-2.45	100.64	107.27
2	A	395	FAD	N9A-C8A-N7A	-2.44	110.47	113.94
2	A	395	FAD	C2'-C1'-N10	2.33	121.20	110.20
2	A	395	FAD	O2-C2-N1	2.31	125.64	121.80
2	A	395	FAD	O2'-C2'-C3'	-2.24	104.01	109.25
2	A	395	FAD	C4X-C10-N10	2.10	119.50	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	O4'-C4'-C5'	-2.05	105.46	109.99
2	A	395	FAD	C4-C4X-C10	2.04	120.43	116.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

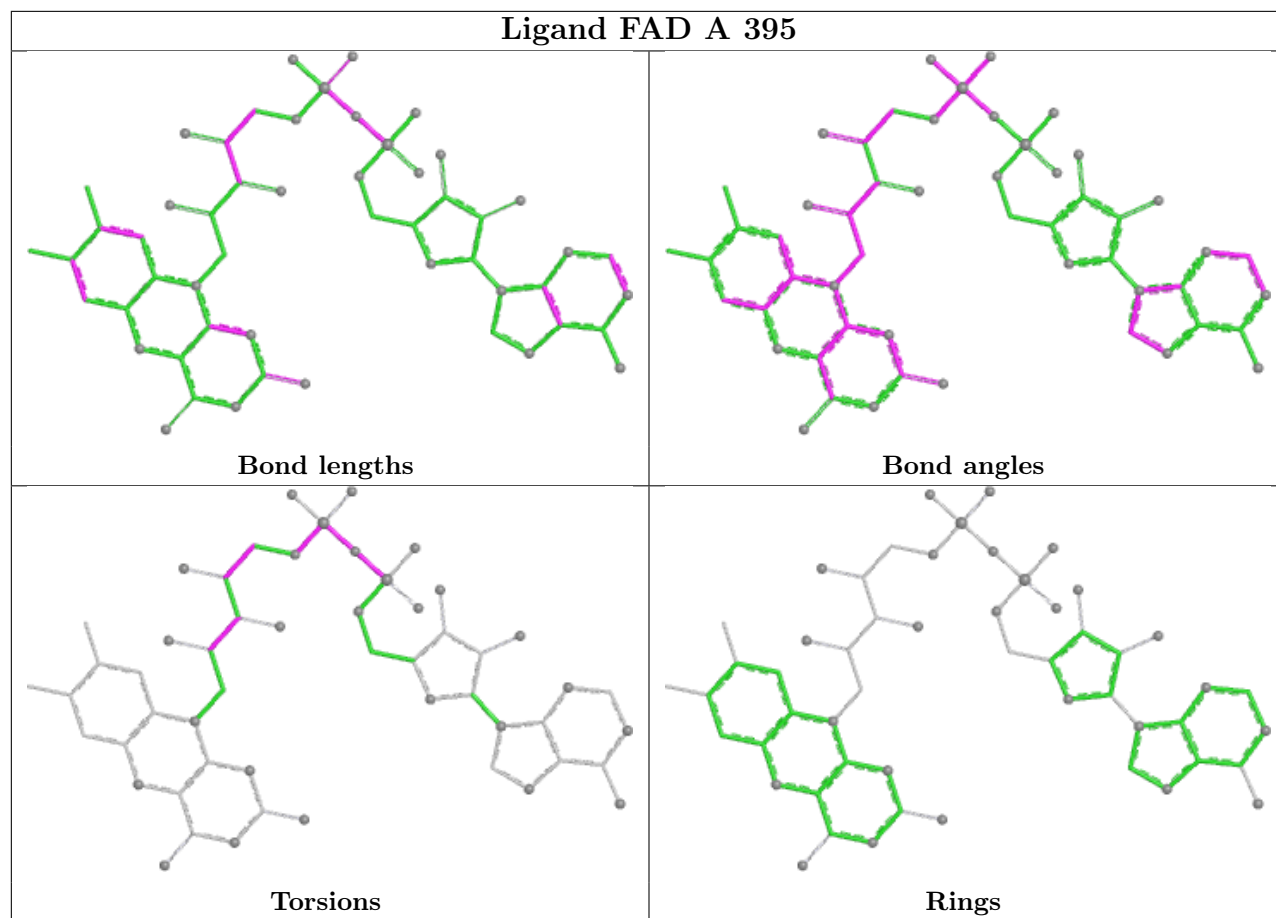
Mol	Chain	Res	Type	Atoms
2	A	395	FAD	C1'-C2'-C3'-O3'
2	A	395	FAD	C1'-C2'-C3'-C4'
2	A	395	FAD	O2'-C2'-C3'-O3'
2	A	395	FAD	O2'-C2'-C3'-C4'
2	A	395	FAD	C3'-C4'-C5'-O5'
2	A	395	FAD	O4'-C4'-C5'-O5'
2	A	395	FAD	C5'-O5'-P-O1P
2	A	395	FAD	C5'-O5'-P-O3P
2	A	395	FAD	PA-O3P-P-O5'
2	A	395	FAD	P-O3P-PA-O2A
2	A	395	FAD	PA-O3P-P-O1P
2	A	395	FAD	PA-O3P-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	395	FAD	1	0
3	A	396	DHB	1	0

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



5.7 Other polymers [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.