



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:19 PM UTC

PDB ID : 1B4U / pdb_00001b4u
Title : PROTOCATECHUATE 4,5-DIOXYGENASE (LIGAB) IN COMPLEX
WITH PROTOCATECHUATE (PCA)
Authors : Sugimoto, K.; Senda, T.; Mitsui, Y.
Deposited on : 1998-12-29
Resolution : 2.20 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
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

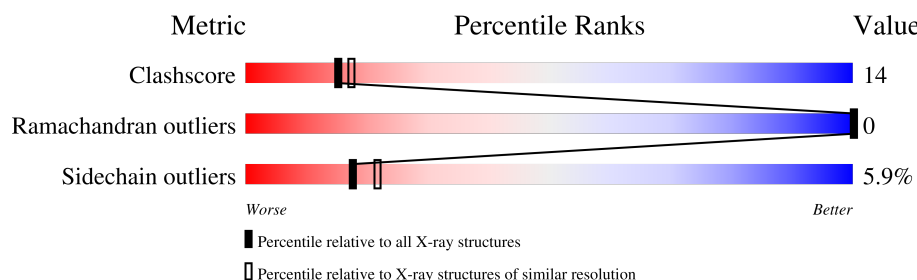
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	139	63% 26% 6% 5%
1	C	139	68% 22% . . 5%
2	B	302	62% 30% 5% . .
2	D	302	61% 30% 6% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6897 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 PROTOCATECHUATE 4,5-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1029	646	177	199	7			
1	C	132	Total	C	N	O	S	0	0	0
			1029	646	177	199	7			

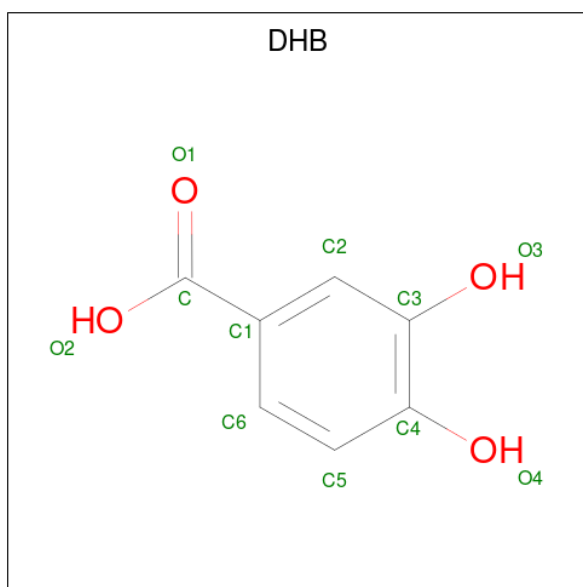
- Molecule 2 is a protein called PROTOCATECHUATE 4,5-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2313	1482	385	430	16			
2	D	298	Total	C	N	O	S	0	0	0
			2313	1482	385	430	16			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is 3,4-DIHYDROXYBENZOIC ACID (CCD ID: DHB) (formula: C₇H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	7	4		
4	D	1	Total	C	O	0	0
			11	7	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	68	Total	O	0	0
			68	68		
5	C	29	Total	O	0	0
			29	29		
5	D	56	Total	O	0	0
			56	56		

3 Residue-property plots [i](#)

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

Note EDS was not executed.

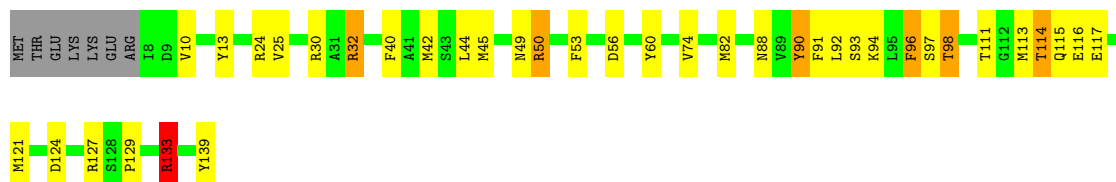
• Molecule 1: PROTOCATECHUATE 4,5-DIOXYGENASE

Chain A:



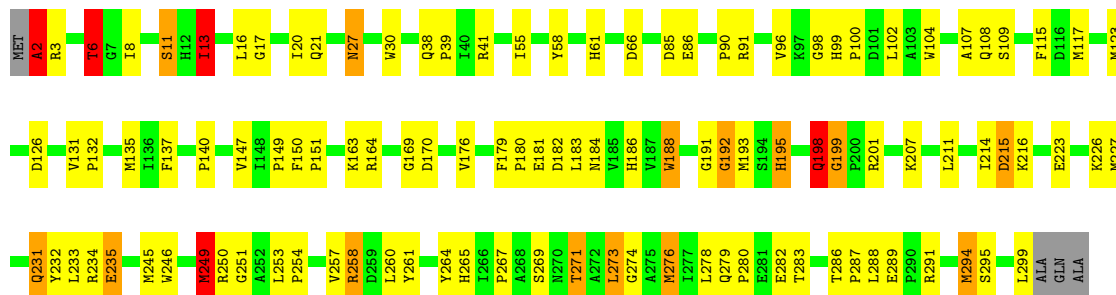
• Molecule 1: PROTOCATECHUATE 4,5-DIOXYGENASE

Chain C:



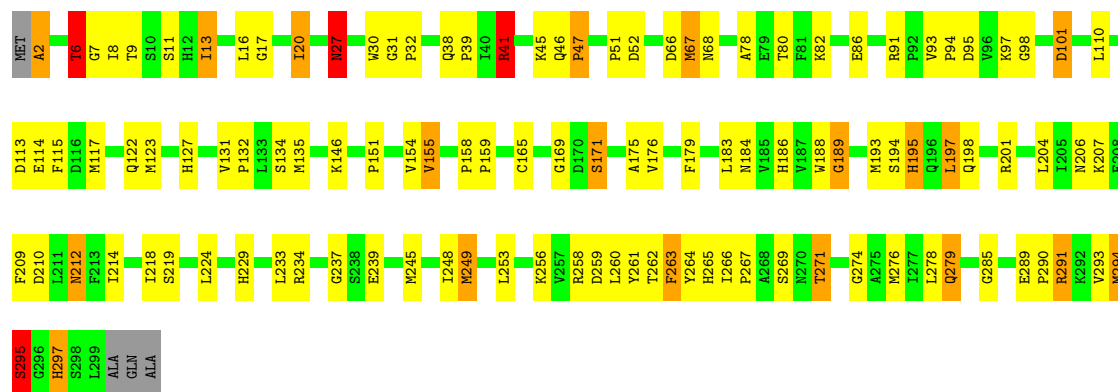
• Molecule 2: PROTOCATECHUATE 4,5-DIOXYGENASE

Chain B:



• Molecule 2: PROTOCATECHUATE 4,5-DIOXYGENASE

Chain D:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.40 Å 66.50 Å 119.80 Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	60.00 – 2.20	Depositor
% Data completeness (in resolution range)	91.0 (60.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6897	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.14	0/1049	2.00	36/1408 (2.6%)
1	C	0.89	0/1049	1.80	19/1408 (1.3%)
2	B	1.15	5/2383 (0.2%)	2.14	89/3253 (2.7%)
2	D	0.99	4/2383 (0.2%)	2.07	67/3253 (2.1%)
All	All	1.06	9/6864 (0.1%)	2.05	211/9322 (2.3%)

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
2	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	ARG	CD-NE	-6.95	1.36	1.46
2	B	249	MET	SD-CE	-6.14	1.64	1.79
2	B	258	ARG	CD-NE	-5.92	1.38	1.46
2	D	245	MET	CG-SD	-5.75	1.66	1.80
2	B	169	GLY	N-CA	5.63	1.52	1.45
2	B	188	TRP	N-CA	5.56	1.52	1.46
2	D	291	ARG	CD-NE	-5.48	1.38	1.46
2	B	91	ARG	CD-NE	-5.32	1.38	1.46
2	D	169	GLY	N-CA	5.01	1.51	1.45

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	291	ARG	CD-NE-CZ	38.16	177.83	124.40
2	B	258	ARG	CD-NE-CZ	24.23	158.33	124.40
2	B	91	ARG	CD-NE-CZ	21.44	154.42	124.40
2	B	41	ARG	CD-NE-CZ	17.62	149.07	124.40
2	D	91	ARG	CD-NE-CZ	15.64	146.29	124.40
2	D	212	ASN	OD1-CG-ND2	12.85	135.45	122.60
2	D	201	ARG	CD-NE-CZ	12.40	141.76	124.40
1	A	96	PHE	CA-CB-CG	12.13	125.93	113.80
2	D	245	MET	CA-CB-CG	-11.48	91.14	114.10
2	D	297	HIS	CA-CB-CG	10.46	124.26	113.80
2	B	215	ASP	CA-CB-CG	-10.14	102.46	112.60
2	D	212	ASN	CA-CB-CG	-10.12	102.47	112.60
2	B	234	ARG	NE-CZ-NH1	9.79	131.29	121.50
1	A	133	ARG	NE-CZ-NH1	9.09	130.59	121.50
2	B	291	ARG	NE-CZ-NH1	-9.05	112.45	121.50
2	D	47	PRO	CA-C-O	-8.69	111.12	121.03
2	B	201	ARG	NE-CZ-NH2	-8.59	111.47	119.20
1	A	19	ASP	CA-C-N	-8.53	116.45	122.59
1	A	19	ASP	C-N-CA	-8.53	116.45	122.59
2	B	257	VAL	CA-C-N	-8.49	110.62	122.93
2	B	257	VAL	C-N-CA	-8.49	110.62	122.93
2	B	41	ARG	NE-CZ-NH2	-8.48	111.56	119.20
2	B	245	MET	CA-CB-CG	-8.46	97.18	114.10
2	B	215	ASP	OD1-CG-OD2	8.32	142.86	122.90
2	B	11	SER	CA-CB-OG	-8.29	94.51	111.10
2	D	201	ARG	NE-CZ-NH2	-8.26	111.77	119.20
2	B	289	GLU	CA-C-O	-8.08	111.79	119.55
2	B	258	ARG	NE-CZ-NH2	-8.00	112.00	119.20
2	B	195	HIS	CA-CB-CG	7.99	121.79	113.80
2	B	41	ARG	CB-CG-CD	7.76	129.15	111.30
2	D	67	MET	CG-SD-CE	7.68	117.80	100.90
2	B	235	GLU	CA-CB-CG	7.61	129.33	114.10
2	B	251	GLY	N-CA-C	-7.59	105.38	115.32
1	A	70	ALA	CA-C-O	7.47	128.54	120.24
2	B	258	ARG	CG-CD-NE	7.46	128.42	112.00
2	D	279	GLN	OE1-CD-NE2	-7.41	115.19	122.60
2	B	85	ASP	CA-C-O	-7.40	112.67	120.58
2	D	154	VAL	CA-C-N	-7.37	113.86	122.63
2	D	154	VAL	C-N-CA	-7.37	113.86	122.63
2	B	294	MET	CA-C-O	-7.32	112.63	120.46
2	B	11	SER	CB-CA-C	7.24	124.51	109.68
2	B	258	ARG	NE-CZ-NH1	7.21	128.71	121.50
2	B	91	ARG	N-CA-CB	7.17	121.24	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	SER	CA-C-N	7.17	126.88	119.56
1	A	128	SER	C-N-CA	7.17	126.88	119.56
2	B	170	ASP	CA-CB-CG	-7.16	105.44	112.60
2	B	91	ARG	CB-CA-C	-7.08	98.34	109.52
2	B	13	ILE	CA-CB-CG2	7.04	122.47	110.50
1	C	96	PHE	CA-CB-CG	7.01	120.81	113.80
2	B	201	ARG	CB-CG-CD	-6.97	95.26	111.30
2	D	184	ASN	CA-C-O	-6.97	113.12	120.58
1	C	50	ARG	CD-NE-CZ	6.93	134.10	124.40
2	D	234	ARG	NE-CZ-NH2	-6.92	112.98	119.20
2	B	3	ARG	N-CA-CB	-6.89	98.80	111.13
2	B	96	VAL	N-CA-CB	-6.88	103.25	110.95
2	D	91	ARG	NE-CZ-NH2	-6.87	113.02	119.20
1	C	97	SER	N-CA-CB	6.81	120.23	110.16
2	D	245	MET	N-CA-C	6.78	119.51	111.71
2	B	41	ARG	NE-CZ-NH1	6.78	128.28	121.50
2	D	101	ASP	CA-C-O	-6.77	113.71	120.82
2	B	109	SER	CA-C-O	-6.74	113.27	120.42
1	A	53	PHE	CA-CB-CG	6.67	120.47	113.80
2	B	276	MET	CA-CB-CG	6.65	127.41	114.10
2	B	249	MET	CG-SD-CE	6.65	115.53	100.90
2	B	91	ARG	NE-CZ-NH1	-6.62	114.88	121.50
2	B	55	ILE	CA-C-N	-6.62	113.71	123.11
2	B	55	ILE	C-N-CA	-6.62	113.71	123.11
1	A	133	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	C	124	ASP	CA-CB-CG	-6.58	106.03	112.60
1	C	98	THR	N-CA-CB	6.56	119.77	110.12
2	B	289	GLU	CB-CA-C	-6.56	101.34	110.13
1	A	48	GLU	CA-C-O	-6.54	113.56	120.63
2	B	2	ALA	N-CA-CB	6.50	120.15	110.40
2	B	11	SER	O-C-N	-6.50	115.38	122.79
1	C	133	ARG	NE-CZ-NH2	-6.49	113.36	119.20
2	B	86	GLU	CA-C-N	-6.40	115.91	123.08
2	B	86	GLU	C-N-CA	-6.40	115.91	123.08
2	B	182	ASP	CA-CB-CG	-6.39	106.21	112.60
2	D	262	THR	CA-C-O	-6.37	112.96	120.60
2	D	263	PHE	CA-CB-CG	6.36	120.16	113.80
1	A	113	MET	N-CA-C	-6.34	100.59	110.42
1	C	40	PHE	CA-C-O	-6.31	114.19	120.82
2	D	97	LYS	CA-C-O	-6.29	113.68	120.92
1	C	53	PHE	N-CA-C	-6.26	104.53	111.36
2	B	164	ARG	CA-C-O	6.26	127.18	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	GLY	CA-C-N	6.25	125.94	119.56
2	B	199	GLY	C-N-CA	6.25	125.94	119.56
2	D	146	LYS	CA-C-O	-6.24	113.88	121.36
2	D	234	ARG	CB-CA-C	-6.22	101.11	110.88
2	D	68	ASN	CA-CB-CG	-6.21	106.39	112.60
2	D	195	HIS	N-CA-C	6.16	117.86	108.07
2	B	198	GLN	OE1-CD-NE2	-6.11	116.50	122.60
2	B	150	PHE	O-C-N	-6.06	115.92	121.37
2	B	17	GLY	N-CA-C	-6.05	105.26	113.37
2	D	234	ARG	CD-NE-CZ	6.03	132.84	124.40
2	B	149	PRO	N-CA-CB	6.02	108.36	103.36
2	D	17	GLY	N-CA-C	-6.02	104.83	113.86
1	A	56	ASP	O-C-N	-6.01	117.97	123.50
1	A	113	MET	CA-C-O	-6.01	114.33	121.66
2	D	201	ARG	NH1-CZ-NH2	5.98	127.08	119.30
2	B	283	THR	N-CA-C	-5.93	104.58	112.94
2	D	41	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	A	52	ARG	CB-CG-CD	5.91	124.90	111.30
1	A	50	ARG	NE-CZ-NH2	5.90	124.51	119.20
2	D	201	ARG	CB-CG-CD	-5.89	97.74	111.30
2	D	210	ASP	CA-C-O	5.85	126.72	120.70
2	B	282	GLU	CA-C-O	-5.83	113.27	119.97
2	B	91	ARG	O-C-N	5.81	127.28	121.30
2	B	192	GLY	CA-C-O	-5.80	115.22	122.65
2	B	234	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	A	66	LEU	CA-C-O	-5.77	114.83	121.47
2	B	273	LEU	CA-C-N	5.75	126.92	121.46
2	B	273	LEU	C-N-CA	5.75	126.92	121.46
2	B	231	GLN	OE1-CD-NE2	-5.74	116.86	122.60
2	B	55	ILE	CA-C-O	-5.71	114.11	120.74
2	B	191	GLY	CA-C-O	-5.71	118.34	122.45
1	A	136	LYS	CA-C-O	-5.70	114.38	120.42
2	D	2	ALA	CA-C-O	-5.70	111.12	120.80
2	B	169	GLY	N-CA-C	-5.69	105.74	113.37
2	B	289	GLU	O-C-N	5.67	128.08	121.10
2	B	215	ASP	N-CA-C	5.67	117.15	110.97
2	B	283	THR	O-C-N	5.67	129.05	122.19
2	B	283	THR	CA-C-O	-5.66	112.80	119.48
2	D	122	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	C	40	PHE	N-CA-C	-5.63	105.04	111.07
1	C	90	TYR	CB-CG-CD2	5.62	129.24	120.80
1	C	32	ARG	CA-CB-CG	-5.61	102.88	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	245	MET	CG-SD-CE	5.61	113.24	100.90
2	D	47	PRO	N-CA-C	-5.59	102.36	110.80
2	D	189	GLY	CA-C-N	-5.59	113.02	123.03
2	D	189	GLY	C-N-CA	-5.59	113.02	123.03
2	B	265	HIS	CA-C-N	5.57	132.43	122.13
2	B	265	HIS	C-N-CA	5.57	132.43	122.13
1	A	35	TYR	O-C-N	-5.56	116.31	122.09
2	D	219	SER	CA-CB-OG	-5.55	99.99	111.10
2	D	294	MET	CA-C-O	-5.55	114.36	120.30
2	D	154	VAL	CA-C-O	-5.54	113.85	120.78
1	A	131	GLY	N-CA-C	-5.50	107.77	114.92
2	D	6	THR	CA-CB-CG2	5.50	119.85	110.50
1	A	16	GLU	CA-C-O	-5.47	113.67	119.97
2	B	107	ALA	CA-C-O	-5.47	115.08	120.82
1	C	56	ASP	CA-C-N	5.44	127.51	120.44
1	C	56	ASP	C-N-CA	5.44	127.51	120.44
2	D	219	SER	CA-C-N	-5.42	116.59	123.15
2	D	219	SER	C-N-CA	-5.42	116.59	123.15
1	A	64	TRP	CA-C-N	-5.42	114.55	122.19
1	A	64	TRP	C-N-CA	-5.42	114.55	122.19
2	D	224	LEU	CA-C-O	5.41	126.19	119.97
2	B	55	ILE	O-C-N	5.40	130.70	122.76
2	D	184	ASN	OD1-CG-ND2	-5.40	117.20	122.60
2	B	108	GLN	OE1-CD-NE2	-5.40	117.20	122.60
2	B	13	ILE	CA-C-O	5.38	124.98	119.82
2	B	245	MET	N-CA-C	5.37	119.09	112.54
1	A	54	LYS	CD-CE-NZ	5.37	129.08	111.90
1	A	128	SER	O-C-N	-5.37	115.42	121.43
2	D	41	ARG	NE-CZ-NH2	-5.37	114.37	119.20
2	D	78	ALA	CA-C-O	5.36	128.09	121.87
2	B	58	TYR	CA-C-O	-5.36	115.71	121.45
2	D	154	VAL	N-CA-CB	5.33	120.02	111.23
2	B	13	ILE	CB-CG1-CD1	-5.32	102.63	113.80
2	D	261	TYR	CA-C-O	-5.32	114.16	120.43
2	B	137	PHE	CA-C-O	-5.31	113.00	119.32
2	D	175	ALA	N-CA-CB	-5.30	102.31	110.16
2	D	258	ARG	CA-C-O	-5.30	114.62	120.30
1	A	127	ARG	CD-NE-CZ	-5.30	116.98	124.40
2	B	140	PRO	CA-C-N	5.29	127.81	120.29
2	B	140	PRO	C-N-CA	5.29	127.81	120.29
2	B	90	PRO	CA-C-O	-5.29	115.55	121.32
1	A	74	VAL	CA-C-N	5.29	127.37	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	VAL	C-N-CA	5.29	127.37	120.28
2	B	126	ASP	CA-CB-CG	5.24	117.84	112.60
2	D	169	GLY	O-C-N	-5.24	116.57	122.28
2	B	246	TRP	N-CA-C	-5.24	105.74	111.82
1	A	105	PHE	CA-CB-CG	-5.22	108.58	113.80
2	B	235	GLU	N-CA-CB	-5.21	102.45	110.42
1	A	45	MET	CA-CB-CG	-5.21	103.68	114.10
1	A	124	ASP	CA-C-N	-5.21	115.29	122.63
1	A	124	ASP	C-N-CA	-5.21	115.29	122.63
1	C	90	TYR	CB-CG-CD1	-5.20	113.00	120.80
2	B	6	THR	CA-CB-OG1	5.19	117.39	109.60
2	D	127	HIS	CA-CB-CG	5.17	118.97	113.80
2	B	184	ASN	OD1-CG-ND2	-5.16	117.44	122.60
2	D	20	ILE	N-CA-CB	5.15	118.31	110.58
1	A	86	GLY	N-CA-C	-5.15	108.13	115.64
2	D	134	SER	CA-C-O	-5.15	115.09	120.55
2	D	2	ALA	N-CA-CB	5.14	118.11	110.40
2	D	155	VAL	CA-CB-CG2	5.14	119.14	110.40
1	C	10	VAL	CA-C-O	-5.14	115.61	120.95
2	D	295	SER	N-CA-CB	5.14	118.75	111.05
2	D	52	ASP	CA-CB-CG	-5.13	107.47	112.60
1	A	124	ASP	CA-C-O	-5.13	112.40	119.12
2	B	100	PRO	O-C-N	-5.12	116.09	122.23
2	D	80	THR	CA-CB-OG1	-5.10	101.95	109.60
2	B	201	ARG	CA-CB-CG	5.09	124.28	114.10
1	C	45	MET	CA-C-O	-5.09	113.12	119.38
1	C	127	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	D	98	GLY	CA-C-N	-5.08	116.17	122.42
2	D	98	GLY	C-N-CA	-5.08	116.17	122.42
2	B	201	ARG	NH1-CZ-NH2	5.08	125.91	119.30
1	C	133	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	27	THR	CA-C-N	5.07	128.43	120.82
1	A	27	THR	C-N-CA	5.07	128.43	120.82
1	A	18	ASP	CA-CB-CG	-5.05	107.55	112.60
2	D	95	ASP	CA-C-N	-5.05	115.85	122.37
2	D	95	ASP	C-N-CA	-5.05	115.85	122.37
2	D	27	ASN	CA-CB-CG	5.05	117.65	112.60
2	D	86	GLU	CA-C-N	-5.04	117.43	123.08
2	D	86	GLU	C-N-CA	-5.04	117.43	123.08
2	B	16	LEU	N-CA-CB	5.04	117.62	110.16
1	C	115	GLN	OE1-CD-NE2	5.04	127.64	122.60
2	B	11	SER	N-CA-CB	-5.00	103.20	110.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2	ALA	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	1029	0	986	20	0
1	C	1029	0	986	33	0
2	B	2313	0	2252	66	0
2	D	2313	0	2252	73	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	11	0	4	3	0
4	D	11	0	4	2	0
5	A	36	0	0	0	0
5	B	68	0	0	0	0
5	C	29	0	0	1	0
5	D	56	0	0	0	0
All	All	6897	0	6484	180	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 14.

All (180) 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)
2:D:7:GLY:HA3	2:D:249:MET:HE3	1.20	1.17
2:D:193:MET:HE1	2:D:214:ILE:HD11	1.32	1.10
1:C:74:VAL:HG22	1:C:82:MET:HE3	1.41	0.97
2:B:193:MET:HE2	2:B:274:GLY:HA3	1.44	0.96
1:C:114:THR:HG22	1:C:117:GLU:HG2	1.47	0.94
2:B:249:MET:HE2	2:B:250:ARG:HA	1.52	0.91
2:B:2:ALA:HB2	2:B:179:PHE:O	1.72	0.90
2:B:193:MET:HE1	2:B:214:ILE:HD11	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ILE:HD11	2:B:135:MET:HE1	1.57	0.86
2:B:115:PHE:HB3	2:B:117:MET:HE3	1.58	0.84
2:D:276:MET:HE2	2:D:278:LEU:HD21	1.61	0.82
2:B:13:ILE:CD1	2:B:269:SER:HB3	2.09	0.81
1:C:24:ARG:H	2:D:198:GLN:HE22	1.30	0.79
1:C:114:THR:HG22	1:C:117:GLU:H	1.48	0.79
2:D:27:ASN:ND2	2:D:30:TRP:H	1.82	0.76
2:D:193:MET:HE2	2:D:274:GLY:HA3	1.66	0.76
2:D:110:LEU:HD13	2:D:117:MET:HE3	1.67	0.76
2:D:193:MET:CE	2:D:274:GLY:HA3	2.17	0.74
2:B:193:MET:CE	2:B:274:GLY:HA3	2.17	0.74
1:C:94:LYS:O	1:C:98:THR:HG23	1.88	0.74
2:B:249:MET:HE2	2:B:250:ARG:CA	2.17	0.74
2:D:16:LEU:HB3	2:D:135:MET:HE3	1.70	0.73
2:D:7:GLY:CA	2:D:249:MET:HE3	2.12	0.70
1:A:24:ARG:H	2:B:198:GLN:HE22	1.37	0.70
2:B:27:ASN:ND2	2:B:30:TRP:H	1.90	0.69
1:A:82:MET:HE2	1:A:92:LEU:HD22	1.73	0.69
2:B:258:ARG:HG2	2:B:260:LEU:HD23	1.75	0.68
2:D:218:ILE:HD11	2:D:276:MET:HE1	1.74	0.68
1:A:82:MET:CE	1:A:92:LEU:HD22	2.23	0.67
2:B:276:MET:HE2	2:B:278:LEU:HD21	1.75	0.67
2:B:249:MET:HE2	2:B:249:MET:C	2.18	0.67
2:B:249:MET:HE2	2:B:250:ARG:N	2.09	0.67
2:B:13:ILE:HD12	2:B:269:SER:HB3	1.76	0.66
2:D:197:LEU:HD22	2:D:239:GLU:HG2	1.77	0.66
2:B:99:HIS:HD2	2:B:102:LEU:H	1.45	0.64
2:B:20:ILE:HD11	2:B:135:MET:CE	2.28	0.64
2:B:216:LYS:HE3	2:B:223:GLU:OE1	1.98	0.64
2:D:271:THR:HG21	4:D:504:DHB:H2	1.80	0.64
2:D:115:PHE:HB3	2:D:117:MET:HE2	1.79	0.63
2:D:6:THR:HB	2:D:279:GLN:HG2	1.81	0.62
2:B:2:ALA:HA	2:B:176:VAL:O	2.01	0.61
2:B:195:HIS:HB3	2:B:271:THR:HB	1.84	0.60
1:C:50:ARG:HD3	1:C:98:THR:HG22	1.84	0.60
2:B:193:MET:HE3	2:B:264:TYR:HD1	1.68	0.59
2:B:27:ASN:HD22	2:B:27:ASN:C	2.11	0.59
2:D:263:PHE:HD1	2:D:293:VAL:HG23	1.68	0.59
2:B:20:ILE:CD1	2:B:135:MET:HE1	2.32	0.58
1:C:129:PRO:O	1:C:133:ARG:HD2	2.03	0.58
1:A:61:LEU:HD21	1:A:74:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:C	2:D:206:ASN:HD22	2.09	0.58
2:B:249:MET:CE	2:B:250:ARG:HA	2.29	0.58
2:D:193:MET:HE3	2:D:264:TYR:HD1	1.68	0.58
2:D:271:THR:HG23	4:D:504:DHB:O1	2.03	0.58
1:A:24:ARG:HH22	1:A:80:ASN:HD22	1.53	0.57
2:B:6:THR:HB	2:B:279:GLN:HG2	1.85	0.57
2:B:271:THR:HG21	4:B:503:DHB:H2	1.87	0.57
2:D:13:ILE:HD12	2:D:269:SER:HB3	1.87	0.57
2:B:115:PHE:HB3	2:B:117:MET:CE	2.33	0.56
2:D:6:THR:HG23	2:D:186:HIS:NE2	2.21	0.55
2:D:16:LEU:HB3	2:D:135:MET:CE	2.35	0.55
1:A:82:MET:HE2	1:A:92:LEU:CD2	2.36	0.55
2:D:115:PHE:CB	2:D:117:MET:HE2	2.36	0.55
2:B:115:PHE:CB	2:B:117:MET:HE3	2.32	0.54
2:D:2:ALA:HA	2:D:176:VAL:O	2.08	0.54
1:C:114:THR:HG22	1:C:117:GLU:CG	2.28	0.54
2:B:211:LEU:HD21	2:B:294:MET:HE1	1.90	0.53
2:B:249:MET:HE2	2:B:249:MET:O	2.08	0.53
2:D:46:GLN:HB3	2:D:47:PRO:CD	2.38	0.53
2:D:51:PRO:HB3	2:D:186:HIS:CD2	2.44	0.53
2:B:193:MET:HE3	2:B:264:TYR:CD1	2.44	0.53
2:D:193:MET:HE1	2:D:214:ILE:CD1	2.22	0.52
2:D:206:ASN:ND2	2:D:209:PHE:H	2.07	0.52
1:A:90:TYR:CE1	2:B:61:HIS:HD2	2.28	0.52
2:B:227:MET:HE3	2:B:232:TYR:CZ	2.44	0.52
1:C:113:MET:HE1	1:C:121:MET:CE	2.40	0.51
2:D:249:MET:HE1	2:D:253:LEU:HD11	1.93	0.51
1:A:74:VAL:HG22	1:A:82:MET:HE3	1.92	0.51
2:B:249:MET:HE3	2:B:253:LEU:CD1	2.41	0.51
2:D:249:MET:HE1	2:D:253:LEU:CD1	2.41	0.50
2:D:27:ASN:HD21	2:D:30:TRP:H	1.55	0.50
2:B:2:ALA:HB3	2:B:181:GLU:O	2.11	0.50
1:C:82:MET:CE	1:C:92:LEU:HD22	2.41	0.50
2:B:131:VAL:HB	2:B:132:PRO:HD3	1.94	0.50
2:D:41:ARG:HD2	2:D:135:MET:O	2.12	0.49
1:C:88:ASN:ND2	1:C:90:TYR:HB2	2.27	0.49
2:D:93:VAL:HB	2:D:94:PRO:HD2	1.93	0.49
2:D:193:MET:HE3	2:D:274:GLY:HA3	1.94	0.49
2:D:207:LYS:HE2	2:D:207:LYS:HB3	1.68	0.48
1:C:114:THR:CG2	1:C:117:GLU:HG2	2.33	0.48
2:B:98:GLY:HA2	2:B:147:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:ILE:HG12	2:D:16:LEU:HG	1.95	0.48
2:D:249:MET:CE	2:D:253:LEU:HD11	2.44	0.48
2:B:271:THR:HG23	4:B:503:DHB:O1	2.13	0.48
1:C:93:SER:HA	1:C:96:PHE:CE2	2.49	0.48
1:A:21:PRO:HG2	1:A:132:VAL:C	2.38	0.48
1:C:44:LEU:HB3	1:C:98:THR:HG21	1.96	0.47
2:B:27:ASN:HD21	2:B:30:TRP:H	1.60	0.47
2:B:123:MET:HE1	2:B:151:PRO:HG3	1.95	0.47
2:D:123:MET:HE1	2:D:151:PRO:HG3	1.96	0.47
2:B:286:THR:HG22	2:B:287:PRO:O	2.14	0.47
2:D:67:MET:HE2	2:D:67:MET:HA	1.95	0.47
1:C:13:TYR:OH	2:D:229:HIS:HD2	1.98	0.47
2:D:276:MET:CE	2:D:278:LEU:HD21	2.39	0.47
2:D:6:THR:HG23	2:D:186:HIS:CD2	2.50	0.47
1:C:24:ARG:H	2:D:198:GLN:NE2	2.06	0.46
1:C:93:SER:HA	1:C:96:PHE:CZ	2.51	0.46
2:D:20:ILE:HD11	2:D:135:MET:HE2	1.97	0.46
1:C:114:THR:H	1:C:117:GLU:CD	2.23	0.46
2:B:271:THR:CG2	4:B:503:DHB:O1	2.63	0.46
1:A:93:SER:HA	1:A:96:PHE:CZ	2.51	0.46
2:D:9:THR:HA	2:D:189:GLY:O	2.16	0.46
1:A:32:ARG:NH2	2:D:101:ASP:OD1	2.47	0.46
1:C:114:THR:H	1:C:117:GLU:CG	2.29	0.45
2:D:131:VAL:HB	2:D:132:PRO:HD3	1.99	0.45
2:B:295:SER:O	2:B:299:LEU:HD12	2.17	0.45
1:C:88:ASN:HD21	1:C:90:TYR:HB2	1.81	0.45
2:B:13:ILE:HD11	2:B:269:SER:HB3	1.97	0.45
2:D:2:ALA:HB2	2:D:179:PHE:O	2.17	0.45
2:D:194:SER:O	2:D:195:HIS:HB3	2.16	0.45
1:C:114:THR:N	1:C:117:GLU:OE2	2.45	0.45
2:B:6:THR:HG23	2:B:186:HIS:NE2	2.32	0.45
1:A:88:ASN:ND2	1:A:90:TYR:H	2.14	0.45
2:D:8:ILE:O	2:D:188:TRP:HA	2.17	0.45
2:D:110:LEU:CD2	2:D:171:SER:HB3	2.47	0.45
2:B:227:MET:HG3	2:B:231:GLN:OE1	2.17	0.45
2:B:99:HIS:CD2	2:B:102:LEU:H	2.30	0.44
2:B:261:TYR:HB2	2:B:288:LEU:HD12	1.99	0.44
1:C:74:VAL:HG22	1:C:82:MET:CE	2.31	0.44
1:A:113:MET:HE2	1:A:127:ARG:HH22	1.82	0.44
2:D:38:GLN:N	2:D:39:PRO:CD	2.80	0.44
2:B:254:PRO:HG2	2:B:280:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:MET:HE2	2:D:66:ASP:HB3	2.00	0.44
1:A:42:MET:HE2	2:B:66:ASP:HB3	2.00	0.44
2:B:216:LYS:HE3	2:B:223:GLU:CD	2.43	0.44
2:B:179:PHE:CD1	2:B:180:PRO:HD2	2.53	0.43
2:B:38:GLN:HB3	2:B:39:PRO:HD3	2.00	0.43
2:D:113:ASP:OD2	2:D:171:SER:OG	2.35	0.43
2:D:290:PRO:HG2	2:D:293:VAL:CG1	2.48	0.43
2:B:294:MET:HE3	2:B:294:MET:HB3	1.94	0.43
2:D:259:ASP:HA	2:D:278:LEU:HD23	2.01	0.43
1:C:82:MET:HE2	1:C:92:LEU:HD22	2.01	0.43
1:C:133:ARG:HD3	1:C:139:TYR:O	2.19	0.43
2:D:265:HIS:ND1	2:D:295:SER:HB2	2.34	0.43
2:D:266:ILE:HA	2:D:267:PRO:HA	1.76	0.43
2:B:273:LEU:C	2:B:273:LEU:HD23	2.44	0.43
1:C:113:MET:HE1	1:C:121:MET:HE1	2.00	0.42
2:D:206:ASN:C	2:D:206:ASN:ND2	2.77	0.42
2:B:13:ILE:HD13	2:B:13:ILE:HG21	1.75	0.42
2:D:279:GLN:HE21	2:D:285:GLY:H	1.67	0.42
2:D:279:GLN:NE2	2:D:285:GLY:H	2.18	0.42
1:A:64:TRP:O	1:A:65:ASN:HB2	2.18	0.42
2:D:218:ILE:HD11	2:D:276:MET:CE	2.47	0.42
2:B:8:ILE:O	2:B:188:TRP:HA	2.20	0.42
1:A:114:THR:OG1	1:A:117:GLU:HG3	2.19	0.42
1:C:91:PHE:CZ	2:D:67:MET:HE3	2.55	0.42
1:A:93:SER:HA	1:A:96:PHE:CE2	2.55	0.42
2:D:7:GLY:HA3	2:D:249:MET:CE	2.15	0.42
2:D:13:ILE:HD12	2:D:269:SER:CB	2.48	0.41
1:A:95:LEU:O	1:A:98:THR:HB	2.19	0.41
1:C:114:THR:HG23	5:C:168:HOH:O	2.20	0.41
2:D:31:GLY:N	2:D:32:PRO:CD	2.83	0.41
1:A:80:ASN:HD21	2:B:199:GLY:HA2	1.85	0.41
1:A:82:MET:HE1	1:A:92:LEU:HD22	1.98	0.41
2:D:165:CYS:HB3	2:D:248:ILE:HG13	2.02	0.41
2:B:192:GLY:HA3	2:B:193:MET:HA	1.89	0.41
2:B:104:TRP:CD1	1:C:32:ARG:HD2	2.56	0.41
1:C:111:THR:OG1	1:C:113:MET:HB2	2.21	0.41
2:D:46:GLN:CB	2:D:47:PRO:CD	2.98	0.41
2:B:223:GLU:HA	2:B:226:LYS:HD2	2.01	0.41
2:D:93:VAL:HB	2:D:94:PRO:CD	2.51	0.41
2:B:211:LEU:HD11	2:B:294:MET:HE1	2.02	0.40
1:C:49:ASN:HB3	1:C:60:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:THR:HG22	2:B:279:GLN:HE21	1.86	0.40
2:B:163:LYS:HD3	2:D:114:GLU:OE2	2.21	0.40
1:C:25:VAL:O	1:C:30:ARG:HD2	2.22	0.40
2:D:289:GLU:HA	2:D:290:PRO:C	2.44	0.40
2:B:258:ARG:HG2	2:B:260:LEU:CD2	2.47	0.40
1:C:88:ASN:ND2	1:C:90:TYR:H	2.19	0.40
2:D:158:PRO:HA	2:D:159:PRO:HD3	1.93	0.40
2:D:204:LEU:HD23	2:D:237:GLY:CA	2.52	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	C	130/139 (94%)	128 (98%)	2 (2%)	0	100	100
2	B	127/302 (42%)	125 (98%)	2 (2%)	0	100	100
2	D	296/302 (98%)	281 (95%)	15 (5%)	0	100	100
All	All	553/743 (74%)	534 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/109 (94%)	98 (96%)	4 (4%)	28	39
1	C	102/109 (94%)	99 (97%)	3 (3%)	37	51
2	B	253/255 (99%)	239 (94%)	14 (6%)	19	24
2	D	253/255 (99%)	232 (92%)	21 (8%)	10	11
All	All	710/728 (98%)	668 (94%)	42 (6%)	18	22

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	16	GLU
1	A	133	ARG
1	A	136	LYS
2	B	6	THR
2	B	11	SER
2	B	13	ILE
2	B	21	GLN
2	B	27	ASN
2	B	183	LEU
2	B	198	GLN
2	B	207	LYS
2	B	215	ASP
2	B	233	LEU
2	B	235	GLU
2	B	249	MET
2	B	267	PRO
2	B	271	THR
1	C	114	THR
1	C	116	GLU
1	C	133	ARG
2	D	6	THR
2	D	11	SER
2	D	13	ILE
2	D	27	ASN
2	D	41	ARG
2	D	45	LYS
2	D	82	LYS
2	D	155	VAL
2	D	171	SER
2	D	183	LEU
2	D	197	LEU
2	D	212	ASN

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Mol	Chain	Res	Type
2	D	233	LEU
2	D	249	MET
2	D	256	LYS
2	D	260	LEU
2	D	271	THR
2	D	291	ARG
2	D	294	MET
2	D	295	SER
2	D	297	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	88	ASN
1	A	104	GLN
1	A	115	GLN
2	B	21	GLN
2	B	27	ASN
2	B	38	GLN
2	B	99	HIS
2	B	121	ASN
2	B	198	GLN
2	B	279	GLN
1	C	88	ASN
1	C	104	GLN
1	C	115	GLN
1	C	120	GLN
2	D	27	ASN
2	D	38	GLN
2	D	121	ASN
2	D	122	GLN
2	D	198	GLN
2	D	206	ASN
2	D	229	HIS
2	D	279	GLN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DHB	D	504	3	11,11,11	1.26	1 (9%)	15,15,15	1.55	3 (20%)
4	DHB	B	503	3	11,11,11	1.02	1 (9%)	15,15,15	2.01	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DHB	D	504	3	-	0/4/4/4	0/1/1/1
4	DHB	B	503	3	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	504	DHB	O3-C3	2.70	1.41	1.36
4	B	503	DHB	C1-C	-2.25	1.44	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	DHB	C6-C1-C2	3.97	123.84	119.25
4	D	504	DHB	O2-C-O1	-3.38	116.08	123.35
4	B	503	DHB	O2-C-O1	-3.22	116.44	123.35
4	B	503	DHB	C5-C4-C3	2.94	122.79	119.66
4	D	504	DHB	O2-C-C1	2.78	121.97	114.84
4	B	503	DHB	C5-C6-C1	-2.48	118.15	120.80
4	D	504	DHB	C2-C3-C4	-2.40	117.67	119.89
4	B	503	DHB	C1-C2-C3	-2.37	118.02	120.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	DHB	2	0
4	B	503	DHB	3	0

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.