



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:11 AM UTC

PDB ID : 1T4P / pdb_00001t4p
Title : Arginase-dehydro-ABH complex
Authors : Cama, E.; Pethe, S.; Boucher, J.-L.; Han, S.; Emig, F.A.; Ash, D.E.; Viola, R.E.; Mansuy, D.; Christianson, D.W.
Deposited on : 2004-04-30
Resolution : 2.60 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

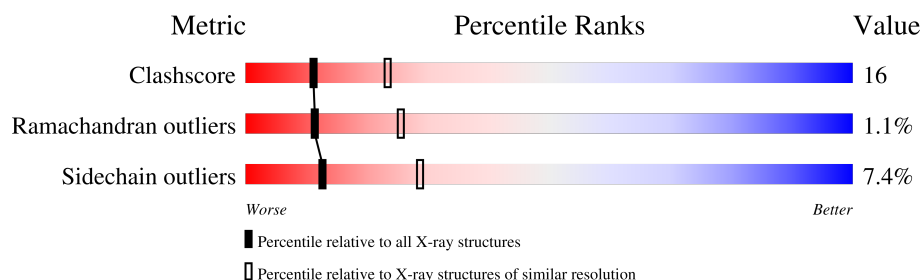
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	314	
1	B	314	
1	C	314	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7338 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.

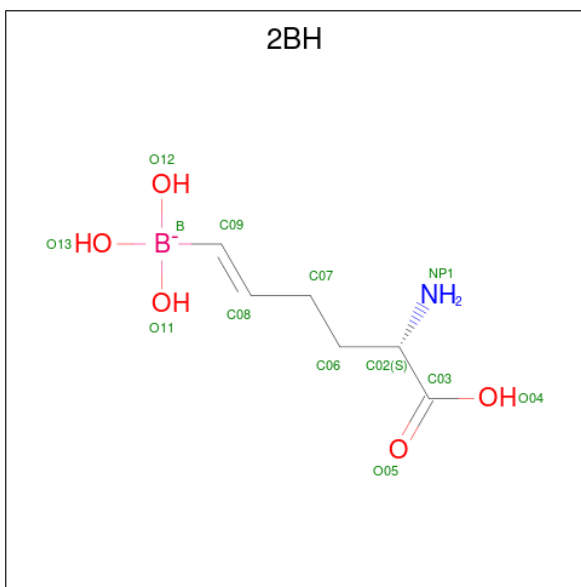
- Molecule 1 is a protein called Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2396	1528	405	456	7			
1	B	314	Total	C	N	O	S	0	0	0
			2396	1528	405	456	7			
1	C	314	Total	C	N	O	S	0	0	0
			2396	1528	405	456	7			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is [(1E,5S)-5-AMINO-5-CARBOXYPENT-1-ENYL](TRIHYDROXY)BORATE (1-) (CCD ID: 2BH) (formula: C₆H₁₃BNO₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			13	1	6	1	5		
3	B	1	Total	B	C	N	O	0	0
			13	1	6	1	5		
3	C	1	Total	B	C	N	O	0	0
			13	1	6	1	5		

- Molecule 4 is water.

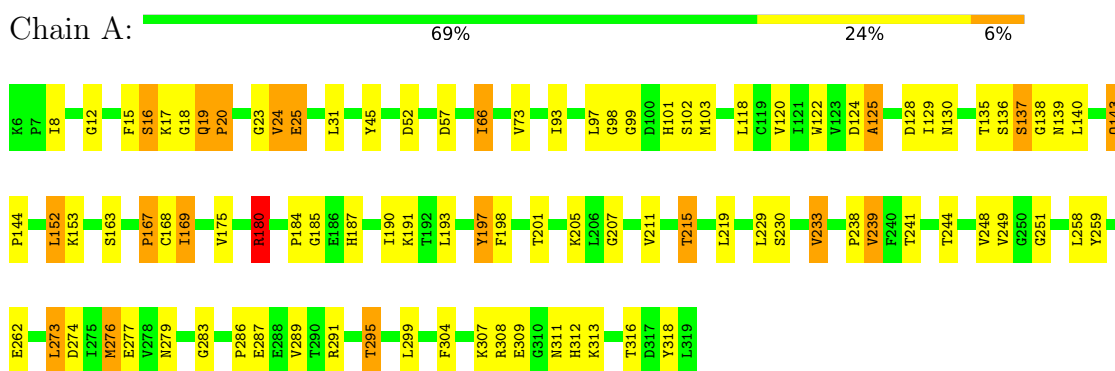
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	55	Total	O	0	0
			55	55		
4	C	21	Total	O	0	0
			21	21		

3 Residue-property plots

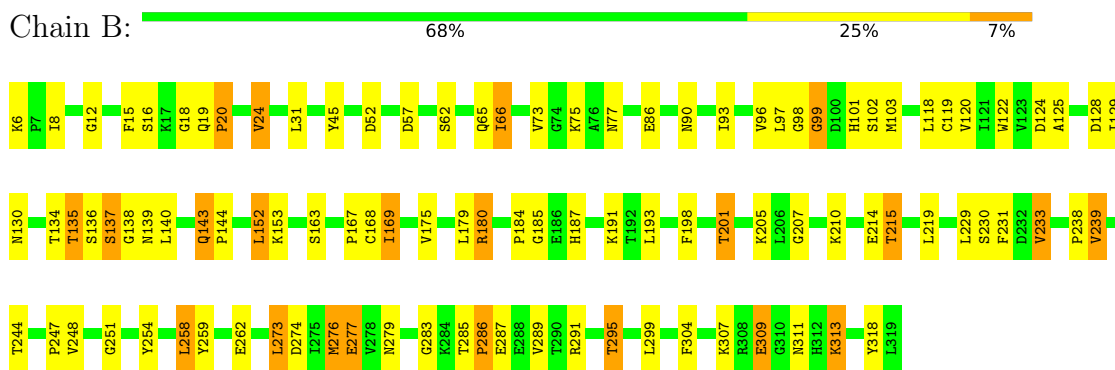
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

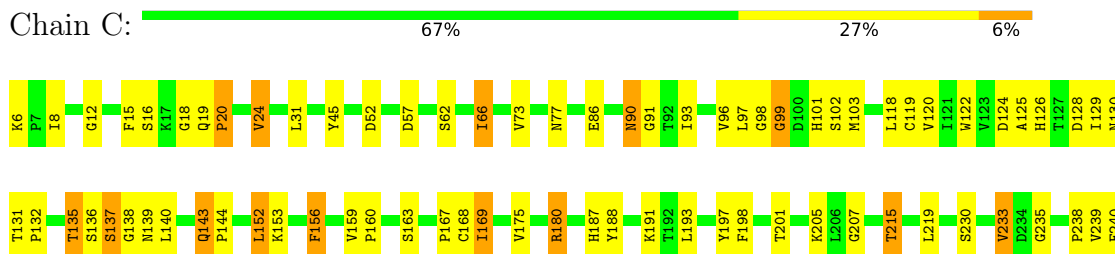
• Molecule 1: Arginase 1

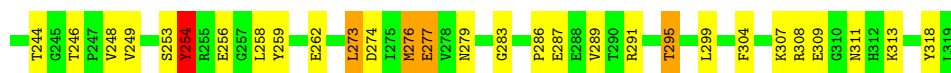


• Molecule 1: Arginase 1



• Molecule 1: Arginase 1





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	88.40 Å 88.40 Å 110.52 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.1 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.264 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7338	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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: 2BH, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	1/2449 (0.0%)	1.07	16/3325 (0.5%)
1	B	0.61	0/2449	1.07	16/3325 (0.5%)
1	C	0.58	0/2449	1.09	19/3325 (0.6%)
All	All	0.60	1/7347 (0.0%)	1.08	51/9975 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	VAL	CA-C	5.38	1.58	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ALA	N-CA-C	-10.36	100.95	114.31
1	C	66	ILE	N-CA-CB	-10.11	101.09	112.21
1	A	125	ALA	N-CA-C	-9.63	101.64	113.97
1	C	125	ALA	N-CA-C	-8.96	102.50	113.97
1	B	66	ILE	N-CA-CB	-8.24	103.15	112.21
1	C	207	GLY	N-CA-C	-8.12	103.20	112.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	GLY	N-CA-C	-7.99	102.81	112.48
1	A	18	GLY	N-CA-C	-7.76	104.76	114.16
1	A	207	GLY	N-CA-C	-7.71	101.84	112.18
1	A	136	SER	N-CA-C	-6.94	102.80	112.45
1	B	276	MET	N-CA-C	6.89	120.27	110.14
1	A	66	ILE	N-CA-CB	-6.77	103.01	112.35
1	A	276	MET	N-CA-C	6.64	119.90	110.14
1	C	276	MET	N-CA-C	6.58	120.19	110.46
1	C	120	VAL	N-CA-C	6.57	117.34	107.75
1	C	279	ASN	CA-C-N	6.36	127.79	119.84
1	C	279	ASN	C-N-CA	6.36	127.79	119.84
1	B	18	GLY	N-CA-C	-6.30	106.54	114.16
1	B	120	VAL	N-CA-C	6.24	116.86	107.75
1	B	309	GLU	N-CA-C	-6.22	105.18	112.89
1	C	136	SER	N-CA-C	-6.21	104.77	112.90
1	A	168	CYS	N-CA-C	5.97	120.63	113.23
1	C	20	PRO	N-CA-C	5.90	121.30	113.57
1	C	246	THR	CA-C-N	5.84	125.85	119.89
1	C	246	THR	C-N-CA	5.84	125.85	119.89
1	A	137	SER	N-CA-C	-5.79	100.75	109.95
1	B	20	PRO	N-CA-C	5.78	121.14	113.57
1	B	279	ASN	CA-C-N	5.75	126.14	119.47
1	B	279	ASN	C-N-CA	5.75	126.14	119.47
1	C	137	SER	N-CA-C	-5.72	100.86	109.95
1	C	309	GLU	N-CA-C	-5.68	105.85	112.89
1	A	20	PRO	N-CA-C	5.65	121.39	113.53
1	B	136	SER	N-CA-C	-5.61	104.66	112.45
1	A	16	SER	N-CA-C	5.60	122.01	112.99
1	C	18	GLY	N-CA-C	-5.60	107.39	114.16
1	B	179	LEU	N-CA-C	5.50	117.99	110.24
1	C	246	THR	N-CA-C	5.36	118.73	108.97
1	B	137	SER	N-CA-C	-5.33	101.47	109.95
1	C	277	GLU	N-CA-C	5.28	119.31	112.86
1	A	309	GLU	N-CA-C	-5.26	106.36	112.89
1	C	254	TYR	N-CA-C	-5.18	105.52	111.07
1	A	279	ASN	CA-C-N	5.16	126.29	119.84
1	A	279	ASN	C-N-CA	5.16	126.29	119.84
1	B	231	PHE	N-CA-C	5.11	116.94	108.20
1	B	277	GLU	N-CA-C	5.10	119.08	112.86
1	B	168	CYS	N-CA-C	5.08	119.75	113.50
1	A	120	VAL	N-CA-C	5.07	115.14	107.75
1	C	131	THR	N-CA-C	-5.04	103.79	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	GLN	CA-C-N	5.01	124.61	119.05
1	A	19	GLN	C-N-CA	5.01	124.61	119.05
1	C	91	GLY	N-CA-C	5.00	121.66	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	GLY	Peptide
1	B	98	GLY	Peptide
1	C	98	GLY	Peptide

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	2396	0	2420	90	0
1	B	2396	0	2420	82	0
1	C	2396	0	2420	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	13	0	11	0	0
3	B	13	0	11	0	0
3	C	13	0	11	0	0
4	A	29	0	0	1	0
4	B	55	0	0	2	0
4	C	21	0	0	3	0
All	All	7338	0	7293	237	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 16.

All (237) 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:318:TYR:HD2	1:B:185:GLY:HA2	1.08	1.11
1:A:318:TYR:CD2	1:B:185:GLY:HA2	1.89	1.07
1:B:175:VAL:HG11	1:B:215:THR:HG22	1.27	1.07
1:C:175:VAL:HG11	1:C:215:THR:HG22	1.29	1.06
1:A:175:VAL:HG11	1:A:215:THR:CG2	1.86	1.06
1:C:132:PRO:HD2	1:C:156:PHE:CD1	1.92	1.05
1:C:132:PRO:HD2	1:C:156:PHE:HD1	1.26	0.98
1:C:175:VAL:HG11	1:C:215:THR:CG2	2.03	0.89
1:A:175:VAL:HG11	1:A:215:THR:HG22	1.52	0.88
1:A:262:GLU:OE1	1:B:201:THR:CG2	2.21	0.88
1:B:175:VAL:HG11	1:B:215:THR:CG2	2.04	0.87
1:C:233:VAL:HG12	1:C:244:THR:HG21	1.59	0.83
1:B:143:GLN:H	1:B:144:PRO:HD3	1.45	0.82
1:A:233:VAL:HG12	1:A:244:THR:HG21	1.62	0.81
1:C:132:PRO:CD	1:C:156:PHE:HD1	1.93	0.81
1:C:132:PRO:CD	1:C:156:PHE:CD1	2.66	0.79
1:B:244:THR:HG22	1:B:277:GLU:O	1.83	0.79
1:A:262:GLU:OE1	1:B:201:THR:HG22	1.84	0.78
1:A:198:PHE:HE1	1:A:215:THR:HG23	1.48	0.77
1:A:135:THR:HB	1:A:137:SER:O	1.85	0.77
1:C:135:THR:HG22	4:C:803:HOH:O	1.83	0.76
1:B:143:GLN:N	1:B:144:PRO:HD3	1.99	0.76
1:C:143:GLN:N	1:C:144:PRO:HD3	2.01	0.75
1:B:262:GLU:OE1	1:C:201:THR:HG22	1.86	0.74
1:A:201:THR:HG22	1:C:262:GLU:OE1	1.88	0.74
1:C:143:GLN:H	1:C:144:PRO:HD3	1.52	0.74
1:B:233:VAL:HG12	1:B:244:THR:HG21	1.69	0.73
1:A:143:GLN:N	1:A:144:PRO:HD3	2.04	0.73
1:B:31:LEU:HD13	1:B:97:LEU:HD22	1.71	0.73
1:C:135:THR:CG2	4:C:803:HOH:O	2.37	0.73
1:A:31:LEU:HD13	1:A:97:LEU:HD22	1.69	0.72
1:A:143:GLN:H	1:A:144:PRO:HD3	1.55	0.72
1:A:311:ASN:O	1:B:184:PRO:HA	1.91	0.71
1:A:197:TYR:HD1	1:A:197:TYR:O	1.74	0.71
1:A:244:THR:HG22	1:A:277:GLU:O	1.91	0.70
1:A:103:MET:HB2	1:A:276:MET:HE1	1.73	0.70
1:A:233:VAL:CG1	1:A:244:THR:HG21	2.21	0.70
1:B:143:GLN:N	1:B:144:PRO:CD	2.54	0.70
1:C:66:ILE:O	1:C:138:GLY:HA3	1.92	0.69
1:B:66:ILE:O	1:B:138:GLY:HA3	1.93	0.68
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.75	0.68
1:C:233:VAL:HG12	1:C:244:THR:CG2	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ASP:HB3	1:C:144:PRO:HD2	1.76	0.67
1:A:128:ASP:HB3	1:A:144:PRO:HD2	1.75	0.67
1:C:143:GLN:N	1:C:144:PRO:CD	2.57	0.67
1:A:143:GLN:N	1:A:144:PRO:CD	2.58	0.67
1:A:230:SER:HA	1:A:274:ASP:HB2	1.78	0.66
1:A:316:THR:HG21	1:A:318:TYR:HE1	1.60	0.66
1:A:66:ILE:O	1:A:138:GLY:HA3	1.95	0.66
1:B:187:HIS:O	1:B:191:LYS:HG2	1.96	0.66
1:A:12:GLY:HA3	1:A:52:ASP:OD1	1.96	0.66
1:C:307:LYS:H	1:C:311:ASN:HD21	1.42	0.66
1:B:180:ARG:NH1	1:B:251:GLY:HA3	2.11	0.65
1:C:12:GLY:HA3	1:C:52:ASP:OD1	1.95	0.65
1:C:244:THR:HG22	1:C:277:GLU:O	1.96	0.65
1:C:198:PHE:CE2	1:C:215:THR:HG23	2.31	0.65
1:A:184:PRO:HA	1:C:311:ASN:O	1.97	0.65
1:B:153:LYS:HD3	1:B:167:PRO:HG2	1.79	0.65
1:A:201:THR:CG2	1:C:262:GLU:OE1	2.46	0.64
1:C:135:THR:HB	1:C:137:SER:O	1.96	0.64
1:A:180:ARG:HG3	1:A:248:VAL:HG11	1.79	0.64
1:C:103:MET:HB2	1:C:276:MET:HE1	1.80	0.64
1:B:103:MET:HB2	1:B:276:MET:HE1	1.81	0.63
1:A:259:TYR:OH	1:B:205:LYS:HD2	1.99	0.63
1:C:273:LEU:HD22	1:C:274:ASP:N	2.13	0.63
1:A:307:LYS:H	1:A:311:ASN:HD21	1.47	0.62
1:B:119:CYS:SG	1:B:219:LEU:HD13	2.39	0.62
1:A:185:GLY:HA2	1:C:318:TYR:CD2	2.35	0.62
1:B:230:SER:HA	1:B:274:ASP:HB2	1.82	0.62
1:A:153:LYS:HD3	1:A:167:PRO:HG2	1.81	0.62
1:A:198:PHE:CE1	1:A:215:THR:HG23	2.32	0.61
1:B:12:GLY:HA3	1:B:52:ASP:OD1	1.99	0.61
1:C:153:LYS:HD3	1:C:167:PRO:HG2	1.82	0.61
1:A:318:TYR:CD2	1:B:185:GLY:CA	2.74	0.61
1:B:233:VAL:HG12	1:B:244:THR:CG2	2.29	0.61
1:A:31:LEU:CD1	1:A:97:LEU:HD22	2.30	0.61
1:A:180:ARG:NH1	1:A:248:VAL:O	2.33	0.61
1:B:273:LEU:HD22	1:B:274:ASP:N	2.17	0.60
1:C:230:SER:HA	1:C:274:ASP:HB2	1.81	0.60
1:A:118:LEU:C	1:A:118:LEU:HD12	2.27	0.60
1:C:31:LEU:HD13	1:C:97:LEU:CD2	2.32	0.60
1:A:316:THR:CG2	1:A:318:TYR:HE1	2.15	0.60
1:A:316:THR:CG2	1:A:318:TYR:CE1	2.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:THR:HB	1:B:137:SER:O	2.02	0.60
1:A:197:TYR:HD1	1:A:197:TYR:C	2.10	0.60
1:B:118:LEU:HD12	1:B:118:LEU:C	2.27	0.60
1:A:273:LEU:HD22	1:A:274:ASP:N	2.16	0.59
1:B:262:GLU:OE1	1:C:201:THR:CG2	2.50	0.59
1:A:197:TYR:C	1:A:197:TYR:CD1	2.81	0.58
1:B:307:LYS:H	1:B:311:ASN:HD21	1.49	0.58
1:B:180:ARG:HG3	1:B:248:VAL:HG11	1.84	0.58
1:A:233:VAL:CG1	1:A:244:THR:CG2	2.80	0.58
1:C:31:LEU:CD1	1:C:97:LEU:HD22	2.33	0.58
1:A:187:HIS:O	1:A:191:LYS:HG2	2.03	0.58
1:A:175:VAL:HG11	1:A:215:THR:HG23	1.83	0.57
1:B:31:LEU:CD1	1:B:97:LEU:HD22	2.34	0.57
1:A:258:LEU:HD23	1:A:299:LEU:HD23	1.87	0.56
1:B:180:ARG:NH1	1:B:251:GLY:CA	2.68	0.56
1:A:318:TYR:O	1:B:134:THR:HG22	2.07	0.55
1:B:180:ARG:NH1	1:B:248:VAL:O	2.39	0.55
1:C:283:GLY:HA3	1:C:289:VAL:HG23	1.89	0.55
1:C:254:TYR:HE1	1:C:258:LEU:HD11	1.71	0.55
1:C:233:VAL:CG1	1:C:244:THR:CG2	2.85	0.55
1:C:169:ILE:HD13	1:C:169:ILE:H	1.72	0.55
1:A:233:VAL:HG12	1:A:244:THR:CG2	2.34	0.55
1:C:187:HIS:O	1:C:191:LYS:HG2	2.06	0.55
1:A:23:GLY:N	1:A:25:GLU:OE2	2.35	0.55
1:B:128:ASP:HA	4:B:791:HOH:O	2.07	0.55
1:A:122:TRP:CD1	1:A:124:ASP:HB2	2.42	0.55
1:C:24:VAL:HB	1:C:99:GLY:HA2	1.89	0.55
1:B:318:TYR:HB2	1:C:188:TYR:CD2	2.43	0.54
1:B:198:PHE:CE2	1:B:215:THR:HG23	2.43	0.54
1:C:180:ARG:HG3	1:C:248:VAL:HG11	1.89	0.54
1:A:8:ILE:HD13	1:A:93:ILE:HB	1.90	0.54
1:A:190:ILE:HD12	1:A:197:TYR:CD2	2.42	0.54
1:B:122:TRP:CD1	1:B:124:ASP:HB2	2.43	0.53
1:A:73:VAL:HG11	1:A:140:LEU:HD13	1.91	0.53
1:A:308:ARG:O	1:B:180:ARG:HA	2.09	0.53
1:A:135:THR:HG21	1:A:143:GLN:NE2	2.23	0.53
1:C:130:ASN:HB3	1:C:135:THR:HG23	1.91	0.53
1:A:259:TYR:CE1	1:B:205:LYS:HB2	2.44	0.53
1:A:283:GLY:HA3	1:A:289:VAL:HG23	1.90	0.52
1:C:233:VAL:CG1	1:C:244:THR:HG21	2.34	0.52
1:C:291:ARG:O	1:C:295:THR:HG22	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:VAL:CG1	1:B:244:THR:HG21	2.38	0.52
4:A:714:HOH:O	1:B:205:LYS:NZ	2.36	0.52
1:B:233:VAL:CG1	1:B:244:THR:CG2	2.87	0.52
1:A:20:PRO:HD3	1:A:139:ASN:OD1	2.09	0.52
1:B:291:ARG:O	1:B:295:THR:HG22	2.10	0.52
1:B:20:PRO:HD3	1:B:139:ASN:OD1	2.10	0.52
1:B:291:ARG:O	1:B:295:THR:CG2	2.57	0.52
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.92	0.52
1:C:86:GLU:O	1:C:90:ASN:ND2	2.43	0.51
1:A:45:TYR:CE2	1:A:304:PHE:HD1	2.28	0.51
1:C:118:LEU:C	1:C:118:LEU:HD12	2.35	0.51
1:C:254:TYR:O	1:C:254:TYR:HD1	1.92	0.51
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.93	0.51
1:C:253:SER:HB2	4:C:716:HOH:O	2.11	0.50
1:B:180:ARG:HD2	1:B:248:VAL:HG12	1.92	0.50
1:C:254:TYR:CD1	1:C:254:TYR:C	2.90	0.50
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.92	0.50
1:B:130:ASN:HB3	1:B:135:THR:HG23	1.93	0.50
1:C:122:TRP:CD1	1:C:124:ASP:HB2	2.46	0.50
1:A:180:ARG:NH1	1:A:251:GLY:HA3	2.27	0.49
1:B:102:SER:HA	1:B:144:PRO:HG3	1.94	0.49
1:C:254:TYR:HD1	1:C:254:TYR:C	2.20	0.49
1:A:16:SER:HB3	1:A:24:VAL:HG23	1.95	0.49
1:C:31:LEU:HD13	1:C:97:LEU:HD22	1.93	0.49
1:A:233:VAL:HG22	1:A:241:THR:HG21	1.94	0.48
1:A:291:ARG:O	1:A:295:THR:CG2	2.61	0.48
1:C:119:CYS:SG	1:C:219:LEU:HD13	2.54	0.48
1:A:15:PHE:HE2	1:A:73:VAL:HG22	1.79	0.48
1:A:180:ARG:NH1	1:A:251:GLY:CA	2.77	0.48
1:A:169:ILE:HD13	1:A:169:ILE:H	1.79	0.48
1:B:96:VAL:HB	1:B:274:ASP:OD1	2.14	0.47
1:B:283:GLY:HA3	1:B:289:VAL:HG23	1.95	0.47
1:A:175:VAL:HG23	1:A:219:LEU:HD21	1.97	0.47
1:B:101:HIS:CE1	1:B:122:TRP:CZ2	3.02	0.47
1:C:45:TYR:CD2	1:C:304:PHE:HB3	2.50	0.47
1:C:180:ARG:NH2	1:C:235:GLY:O	2.48	0.47
1:B:180:ARG:CZ	1:B:251:GLY:HA3	2.45	0.47
1:C:273:LEU:CD2	1:C:274:ASP:N	2.77	0.47
1:C:20:PRO:HD3	1:C:139:ASN:OD1	2.14	0.47
1:A:124:ASP:OD1	1:A:125:ALA:N	2.48	0.47
1:B:254:TYR:CE2	1:C:249:VAL:HG23	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:HD23	1:C:299:LEU:HD23	1.97	0.46
1:A:198:PHE:CD1	1:A:211:VAL:HG13	2.49	0.46
1:C:291:ARG:O	1:C:295:THR:CG2	2.63	0.46
1:A:135:THR:HG21	1:A:143:GLN:CD	2.40	0.46
1:C:31:LEU:HD12	1:C:97:LEU:HD22	1.98	0.46
1:C:175:VAL:HG23	1:C:219:LEU:HD21	1.96	0.46
1:A:312:HIS:HA	1:B:184:PRO:HB3	1.97	0.46
1:C:240:PHE:CE2	1:C:253:SER:HA	2.50	0.46
1:B:24:VAL:HB	1:B:99:GLY:HA2	1.98	0.46
1:A:291:ARG:O	1:A:295:THR:HG22	2.16	0.46
1:C:102:SER:HA	1:C:144:PRO:HG3	1.97	0.46
1:A:180:ARG:HA	1:C:308:ARG:O	2.16	0.45
1:C:15:PHE:HE2	1:C:73:VAL:HG22	1.80	0.45
1:A:102:SER:HA	1:A:144:PRO:HG3	1.98	0.45
1:B:15:PHE:HE2	1:B:73:VAL:HG22	1.80	0.45
1:B:77:ASN:OD1	1:B:103:MET:HA	2.17	0.45
1:C:90:ASN:H	1:C:90:ASN:HD22	1.64	0.45
1:C:156:PHE:N	1:C:156:PHE:CD2	2.84	0.45
1:C:156:PHE:N	1:C:156:PHE:HD2	2.15	0.45
1:A:259:TYR:CZ	1:B:205:LYS:HB2	2.52	0.45
1:B:309:GLU:HB2	1:C:197:TYR:HE2	1.81	0.44
1:A:130:ASN:HB3	1:A:135:THR:CG2	2.47	0.44
1:A:316:THR:HG22	1:A:318:TYR:CD1	2.52	0.44
1:A:101:HIS:CE1	1:A:122:TRP:CZ2	3.06	0.44
1:A:190:ILE:HD12	1:A:197:TYR:HD2	1.82	0.44
1:B:86:GLU:O	1:B:90:ASN:ND2	2.51	0.44
1:A:45:TYR:CE2	1:A:304:PHE:CD1	3.05	0.44
1:C:16:SER:HB3	1:C:24:VAL:HG23	2.00	0.43
1:B:20:PRO:HD3	1:B:139:ASN:CG	2.43	0.43
1:C:73:VAL:HG11	1:C:140:LEU:HD13	2.00	0.43
1:A:19:GLN:HB2	1:A:20:PRO:HD2	2.01	0.43
1:B:8:ILE:HD13	1:B:93:ILE:HB	1.99	0.43
1:B:16:SER:HB3	1:B:24:VAL:HG23	1.99	0.43
1:B:45:TYR:CD2	1:B:304:PHE:HB3	2.54	0.43
1:C:8:ILE:HD13	1:C:93:ILE:HB	2.01	0.43
1:B:129:ILE:HG12	1:B:129:ILE:O	2.19	0.43
1:B:258:LEU:HD23	1:B:299:LEU:HD23	2.01	0.43
1:C:101:HIS:HA	1:C:276:MET:HE3	2.01	0.43
1:A:20:PRO:HD3	1:A:139:ASN:CG	2.45	0.42
1:A:205:LYS:HB2	1:C:259:TYR:CE1	2.55	0.42
1:B:19:GLN:HB2	1:B:20:PRO:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ILE:HG12	1:C:129:ILE:O	2.19	0.42
1:B:75:LYS:HA	1:B:75:LYS:HD2	1.85	0.42
1:B:259:TYR:CE1	1:C:205:LYS:HB2	2.54	0.42
1:C:126:HIS:HB2	1:C:128:ASP:OD1	2.19	0.42
1:C:19:GLN:HB2	1:C:20:PRO:HD2	2.00	0.42
1:B:239:VAL:O	1:B:239:VAL:CG1	2.68	0.42
1:B:313:LYS:HB2	1:B:313:LYS:HE3	1.81	0.42
1:C:96:VAL:HB	1:C:274:ASP:OD1	2.20	0.42
1:C:101:HIS:CE1	1:C:122:TRP:CZ2	3.08	0.42
1:A:229:LEU:O	1:A:273:LEU:HD23	2.20	0.42
1:A:239:VAL:O	1:A:239:VAL:CG1	2.67	0.42
1:C:273:LEU:CD2	1:C:274:ASP:H	2.33	0.42
1:A:31:LEU:HD13	1:A:97:LEU:CD2	2.43	0.41
1:A:316:THR:HG22	1:A:318:TYR:CE1	2.55	0.41
1:B:73:VAL:HG11	1:B:140:LEU:HD13	2.01	0.41
1:A:130:ASN:HB3	1:A:135:THR:HG23	2.01	0.41
1:B:229:LEU:O	1:B:273:LEU:HD23	2.21	0.41
1:C:132:PRO:CG	1:C:156:PHE:HD1	2.34	0.41
1:A:129:ILE:HG12	1:A:129:ILE:O	2.21	0.41
1:B:247:PRO:HA	4:B:752:HOH:O	2.19	0.41
1:C:180:ARG:HD2	1:C:248:VAL:HG12	2.01	0.41
1:C:253:SER:OG	1:C:256:GLU:HG3	2.21	0.41
1:B:169:ILE:HD13	1:B:169:ILE:H	1.85	0.41
1:B:210:LYS:HE3	1:B:214:GLU:OE2	2.21	0.40
1:C:77:ASN:OD1	1:C:103:MET:HA	2.21	0.40
1:B:101:HIS:HA	1:B:276:MET:HE3	2.02	0.40
1:B:285:THR:O	1:B:286:PRO:C	2.63	0.40
1:C:66:ILE:HD13	1:C:66:ILE:HG21	1.89	0.40
1:C:90:ASN:ND2	1:C:90:ASN:H	2.19	0.40
1:C:159:VAL:HA	1:C:160:PRO:HD3	1.95	0.40
1:A:8:ILE:HD11	1:A:45:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

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	312/314 (99%)	293 (94%)	15 (5%)	4 (1%)	9	21
1	B	312/314 (99%)	292 (94%)	17 (5%)	3 (1%)	12	28
1	C	312/314 (99%)	292 (94%)	17 (5%)	3 (1%)	12	28
All	All	936/942 (99%)	877 (94%)	49 (5%)	10 (1%)	11	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLY
1	B	99	GLY
1	C	99	GLY
1	A	180	ARG
1	C	180	ARG
1	B	180	ARG
1	A	143	GLN
1	B	143	GLN
1	C	143	GLN
1	A	167	PRO

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	264/264 (100%)	246 (93%)	18 (7%)	14	32
1	B	264/264 (100%)	244 (92%)	20 (8%)	12	27
1	C	264/264 (100%)	243 (92%)	21 (8%)	11	25
All	All	792/792 (100%)	733 (93%)	59 (7%)	13	29

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	24	VAL
1	A	25	GLU
1	A	57	ASP
1	A	152	LEU
1	A	163	SER
1	A	169	ILE
1	A	180	ARG
1	A	197	TYR
1	A	215	THR
1	A	233	VAL
1	A	238	PRO
1	A	239	VAL
1	A	273	LEU
1	A	286	PRO
1	A	287	GLU
1	A	295	THR
1	A	313	LYS
1	B	6	LYS
1	B	24	VAL
1	B	57	ASP
1	B	62	SER
1	B	65	GLN
1	B	135	THR
1	B	152	LEU
1	B	163	SER
1	B	169	ILE
1	B	201	THR
1	B	215	THR
1	B	233	VAL
1	B	238	PRO
1	B	239	VAL
1	B	258	LEU
1	B	273	LEU
1	B	286	PRO
1	B	287	GLU
1	B	295	THR
1	B	313	LYS
1	C	6	LYS
1	C	24	VAL
1	C	57	ASP
1	C	62	SER
1	C	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	135	THR
1	C	152	LEU
1	C	156	PHE
1	C	163	SER
1	C	168	CYS
1	C	169	ILE
1	C	215	THR
1	C	233	VAL
1	C	238	PRO
1	C	239	VAL
1	C	254	TYR
1	C	273	LEU
1	C	286	PRO
1	C	287	GLU
1	C	295	THR
1	C	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	311	ASN
1	B	79	GLN
1	B	143	GLN
1	B	311	ASN
1	C	90	ASN
1	C	143	GLN
1	C	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2BH	C	1002	2	10,12,12	3.02	6 (60%)	9,16,16	1.05	0
3	2BH	A	1000	2	10,12,12	2.94	6 (60%)	9,16,16	1.09	1 (11%)
3	2BH	B	1001	2	10,12,12	2.77	6 (60%)	9,16,16	1.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2BH	C	1002	2	-	0/8/12/12	-
3	2BH	A	1000	2	-	0/8/12/12	-
3	2BH	B	1001	2	-	0/8/12/12	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	2BH	O05-C03	5.29	1.37	1.22
3	A	1000	2BH	B-O13	-4.77	1.39	1.48
3	C	1002	2BH	B-C09	-4.55	1.52	1.58
3	A	1000	2BH	O05-C03	4.47	1.35	1.22
3	B	1001	2BH	B-O13	-4.39	1.39	1.48
3	A	1000	2BH	B-C09	-4.34	1.52	1.58
3	C	1002	2BH	B-O13	-4.29	1.39	1.48
3	B	1001	2BH	O05-C03	3.89	1.33	1.22
3	B	1001	2BH	B-O11	-3.64	1.41	1.48
3	B	1001	2BH	B-C09	-3.45	1.53	1.58
3	C	1002	2BH	B-O11	-3.08	1.42	1.48
3	A	1000	2BH	B-O11	-3.05	1.42	1.48
3	B	1001	2BH	O04-C03	-2.87	1.21	1.30
3	B	1001	2BH	B-O12	-2.82	1.42	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	2BH	O04-C03	-2.76	1.21	1.30
3	A	1000	2BH	B-O12	-2.72	1.42	1.48
3	C	1002	2BH	B-O12	-2.30	1.43	1.48
3	C	1002	2BH	O04-C03	-2.19	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	2BH	O13-B-O12	-2.03	101.17	108.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.