



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2026 – 12:01 PM EDT

PDB ID : 1DV1 / pdb_00001dv1
Title : STRUCTURE OF BIOTIN CARBOXYLASE (APO)
Authors : Thoden, J.B.; Blanchard, C.Z.; Holden, H.M.; Waldrop, G.L.
Deposited on : 2000-01-19
Resolution : 1.90 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)	:	2.50

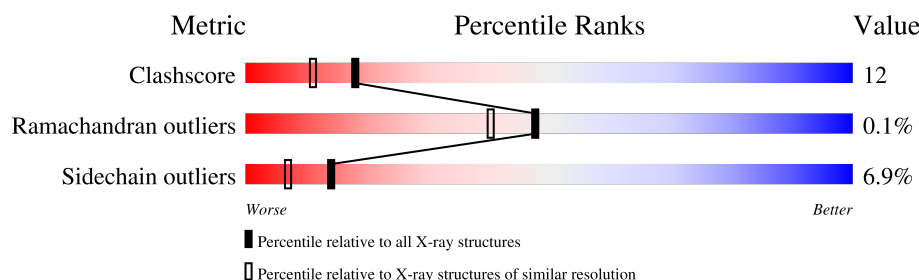
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	449	
1	B	449	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1000	-	X	-	-

2 Entry composition [i](#)

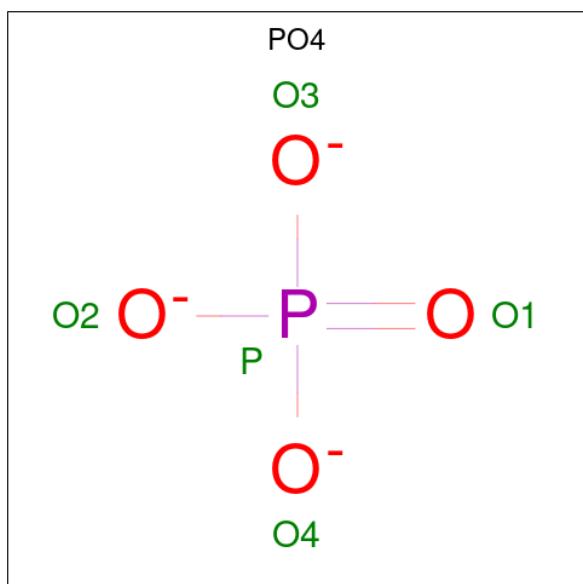
There are 3 unique types of molecules in this entry. The entry contains 7197 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BIOTIN CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	2	0
			3361	2122	595	623	21			
1	B	428	Total	C	N	O	S	0	2	0
			3282	2077	582	605	18			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	300	Total 300	O 300	0	0
3	B	244	Total 244	O 244	0	0

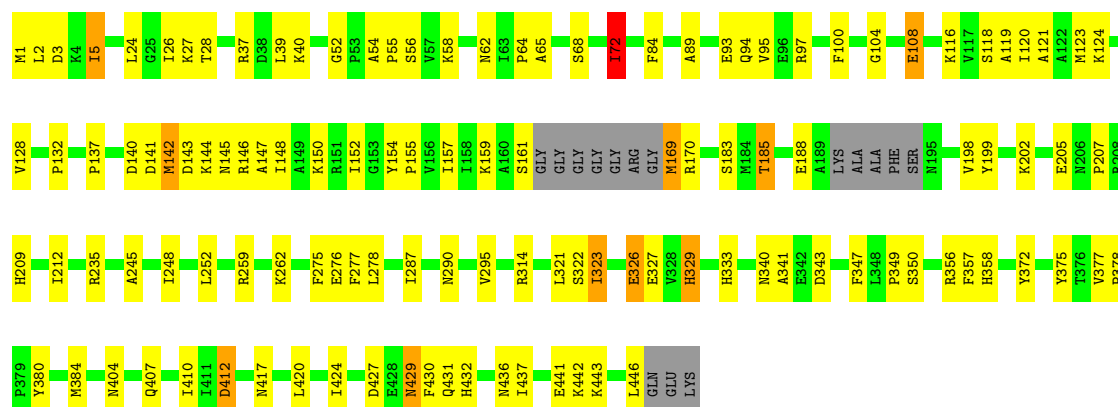
3 Residue-property plots

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.

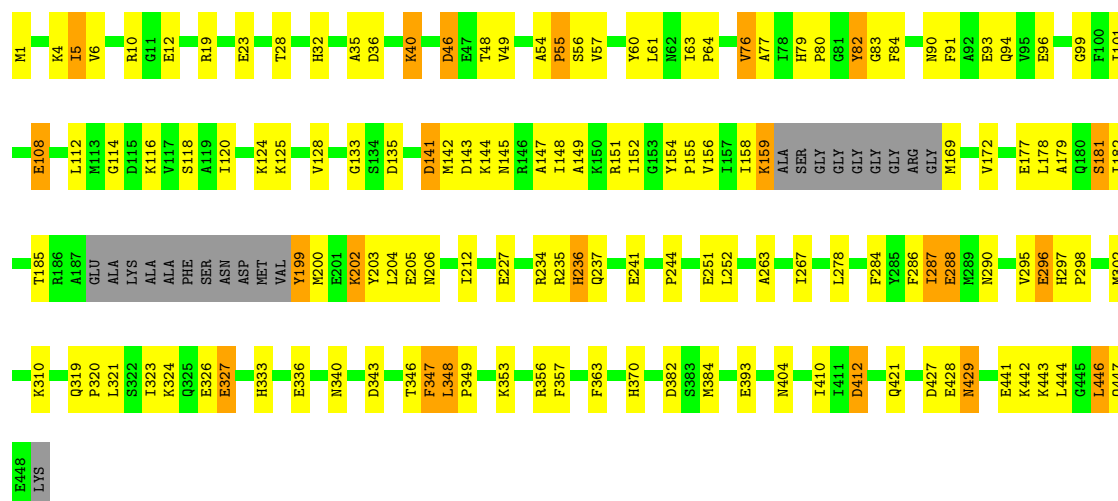
• Molecule 1: BIOTIN CARBOXYLASE

Chain A: 



• Molecule 1: BIOTIN CARBOXYLASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.70Å 95.80Å 180.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	92.1 (30.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.180 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7197	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: PO4

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	1.24	4/3429 (0.1%)	1.63	35/4629 (0.8%)
1	B	1.23	3/3351 (0.1%)	1.63	33/4532 (0.7%)
All	All	1.23	7/6780 (0.1%)	1.63	68/9161 (0.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CD-OE2	7.26	1.39	1.25
1	A	350	SER	N-CA	-6.08	1.40	1.46
1	B	441	GLU	C-N	-5.38	1.26	1.33
1	A	39	LEU	CA-C	-5.20	1.46	1.52
1	A	358	HIS	CE1-NE2	5.12	1.37	1.32
1	B	288	GLU	CA-C	-5.04	1.46	1.52
1	B	326	GLU	CD-OE2	5.04	1.34	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	PHE	CA-CB-CG	-9.98	103.82	113.80
1	A	329	HIS	CA-CB-CG	-9.52	104.28	113.80
1	A	380	TYR	N-CA-C	8.63	121.63	111.71
1	A	358	HIS	CA-CB-CG	-8.45	105.35	113.80
1	A	350	SER	CA-C-N	8.08	128.03	120.03
1	A	350	SER	C-N-CA	8.08	128.03	120.03
1	A	378	PRO	N-CA-CB	7.70	107.22	103.22
1	B	287	ILE	CB-CA-C	-7.68	105.18	111.71
1	A	429	ASN	CA-CB-CG	-7.52	105.08	112.60
1	B	290	ASN	CA-CB-CG	-7.32	105.28	112.60
1	A	275	PHE	CA-CB-CG	-7.25	106.56	113.80
1	B	46	ASP	CA-CB-CG	-7.24	105.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	PRO	N-CA-CB	6.94	109.43	103.19
1	A	430	PHE	CA-CB-CG	-6.92	106.88	113.80
1	A	377	VAL	CA-C-N	6.76	124.53	119.66
1	A	377	VAL	C-N-CA	6.76	124.53	119.66
1	B	91	PHE	CA-CB-CG	-6.74	107.06	113.80
1	A	349	PRO	N-CA-CB	6.59	108.85	103.32
1	A	52	GLY	CA-C-N	6.36	126.32	120.21
1	A	52	GLY	C-N-CA	6.36	126.32	120.21
1	B	347	PHE	CA-CB-CG	-6.35	107.45	113.80
1	B	370	HIS	CA-CB-CG	-6.34	107.46	113.80
1	B	429	ASN	CA-CB-CG	-6.28	106.32	112.60
1	B	236	HIS	CA-CB-CG	-6.18	107.62	113.80
1	A	437	ILE	N-CA-C	5.90	120.67	113.00
1	A	407	GLN	N-CA-CB	5.85	119.35	110.28
1	A	205	GLU	N-CA-C	5.79	117.39	111.14
1	B	12	GLU	N-CA-C	5.79	117.26	111.07
1	A	84	PHE	CA-CB-CG	-5.69	108.11	113.80
1	A	432	HIS	N-CA-C	-5.59	105.26	111.36
1	A	287	ILE	CB-CA-C	-5.59	102.12	111.29
1	B	412	ASP	CA-C-N	-5.55	117.41	123.30
1	B	412	ASP	C-N-CA	-5.55	117.41	123.30
1	A	124	LYS	CA-C-N	5.51	127.98	120.54
1	A	124	LYS	C-N-CA	5.51	127.98	120.54
1	A	3	ASP	N-CA-C	5.47	118.08	111.40
1	B	287	ILE	N-CA-C	-5.43	106.38	111.48
1	B	412	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	135[A]	ASP	N-CA-C	-5.39	104.61	110.91
1	B	135[B]	ASP	N-CA-C	-5.39	104.61	110.91
1	B	349	PRO	CA-C-N	-5.32	117.00	122.85
1	B	349	PRO	C-N-CA	-5.32	117.00	122.85
1	B	206	ASN	CA-CB-CG	-5.31	107.29	112.60
1	B	12	GLU	CA-C-O	5.25	126.33	120.82
1	B	143	ASP	N-CA-C	-5.23	105.64	112.23
1	B	296	GLU	N-CA-C	5.19	119.33	113.15
1	B	128	VAL	CA-C-N	5.19	126.00	119.98
1	B	128	VAL	C-N-CA	5.19	126.00	119.98
1	B	6	VAL	N-CA-CB	5.17	117.19	110.99
1	A	28	THR	N-CA-C	5.15	118.20	109.76
1	A	341	ALA	CA-C-N	-5.15	113.87	122.21
1	A	341	ALA	C-N-CA	-5.15	113.87	122.21
1	B	114	GLY	CA-C-N	-5.14	115.93	122.77
1	B	114	GLY	C-N-CA	-5.14	115.93	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	132	PRO	N-CA-CB	5.09	108.06	103.33
1	A	72	ILE	CB-CA-C	-5.09	104.28	112.16
1	B	108	GLU	N-CA-CB	5.08	117.58	110.12
1	A	137	PRO	N-CA-CB	5.08	108.16	103.39
1	B	363	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	417	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	275	PHE	CB-CA-C	-5.04	102.03	110.19
1	B	32	HIS	N-CA-C	5.04	116.72	109.07
1	A	169	MET	N-CA-CB	5.03	119.06	110.50
1	A	377	VAL	O-C-N	5.03	126.83	121.10
1	A	295	VAL	CB-CA-C	-5.02	105.45	111.88
1	B	82	TYR	N-CA-CB	5.01	120.27	111.55
1	B	349	PRO	N-CA-CB	5.01	108.51	103.25

There are no chirality outliers.

There are no planarity outliers.

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	3361	0	3374	62	0
1	B	3282	0	3264	100	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	300	0	0	10	0
3	B	244	0	0	9	0
All	All	7197	0	6638	162	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 12.

All (162) 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:B:149:ALA:HA	1:B:200:MET:HE1	1.30	1.11
1:B:152:ILE:HD12	1:B:200:MET:HE2	1.33	1.06
1:B:235:ARG:HH12	1:B:446:LEU:HB3	1.22	1.01
1:A:185:THR:HG22	1:A:198:VAL:HG11	1.56	0.87
1:B:152:ILE:HD12	1:B:200:MET:CE	2.04	0.87
1:B:177:GLU:O	1:B:181:SER:HB2	1.76	0.84
1:A:427:ASP:O	1:A:431:GLN:HG3	1.82	0.79
1:A:150:LYS:HB2	3:A:1283:HOH:O	1.84	0.76
1:B:203:TYR:CE2	1:B:205:GLU:HG3	2.21	0.76
1:A:94:GLN:HG3	1:A:97:ARG:NH2	2.01	0.75
1:B:120:ILE:HG22	1:B:124:LYS:HD2	1.69	0.73
1:B:340:ASN:HD22	1:B:384:MET:HA	1.55	0.71
1:B:112:LEU:HD12	1:B:118:SER:HB2	1.73	0.71
1:A:27:LYS:HE2	3:A:1500:HOH:O	1.89	0.71
1:A:427:ASP:OD1	1:A:443:LYS:HE3	1.92	0.70
1:B:149:ALA:CA	1:B:200:MET:HE1	2.16	0.69
1:A:62:ASN:OD1	1:A:64:PRO:HD2	1.92	0.69
1:A:333:HIS:ND1	3:A:1243:HOH:O	2.26	0.69
1:B:152:ILE:CD1	1:B:200:MET:HE2	2.19	0.68
1:B:203:TYR:HE2	1:B:205:GLU:HG3	1.58	0.66
1:A:185:THR:HG22	1:A:198:VAL:CG1	2.25	0.66
1:B:324:LYS:O	1:B:327:GLU:HG3	1.97	0.65
1:B:159:LYS:HB2	1:B:199:TYR:HE1	1.61	0.64
1:B:158:ILE:HG22	1:B:185:THR:HG21	1.79	0.63
1:B:428:GLU:HB2	3:B:1511:HOH:O	1.98	0.62
1:B:152:ILE:HG23	1:B:202:LYS:HB2	1.81	0.61
1:A:343:ASP:O	1:A:347:PHE:N	2.29	0.60
1:B:235:ARG:NH1	1:B:446:LEU:HB3	2.05	0.60
1:B:404:ASN:ND2	3:B:1376:HOH:O	2.32	0.60
1:A:212:ILE:HD13	1:A:277:PHE:CE1	2.37	0.59
1:A:94:GLN:HG3	1:A:97:ARG:CZ	2.33	0.58
1:B:159:LYS:CB	1:B:199:TYR:HE1	2.15	0.58
1:A:340:ASN:HD22	1:A:384:MET:HA	1.69	0.58
1:A:245:ALA:HB3	1:A:248:ILE:HG13	1.86	0.57
1:A:326:GLU:HG2	3:A:1301:HOH:O	2.03	0.57
1:B:427:ASP:OD2	1:B:429:ASN:HB2	2.04	0.57
1:B:159:LYS:HG2	1:B:169:MET:CB	2.35	0.57
1:A:68:SER:O	1:A:72:ILE:HG13	2.04	0.56
1:B:158:ILE:HD11	1:B:172:VAL:HG21	1.86	0.56
1:B:56:SER:O	1:B:61:LEU:N	2.32	0.56
1:A:118:SER:O	1:A:121:ALA:HB3	2.06	0.56
1:B:154:TYR:HB3	1:B:155:PRO:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB3	3:A:1642:HOH:O	2.06	0.56
1:A:152:ILE:HG23	1:A:202:LYS:HB2	1.88	0.55
1:A:356:ARG:NE	1:A:412:ASP:OD1	2.33	0.55
1:A:94:GLN:HG2	1:A:97:ARG:NH1	2.21	0.55
1:A:185:THR:CG2	1:A:198:VAL:HG11	2.35	0.54
1:B:159:LYS:HB2	1:B:199:TYR:CE1	2.41	0.54
1:B:96:GLU:O	1:B:99:GLY:N	2.35	0.52
1:B:179:ALA:HB3	3:B:1532:HOH:O	2.09	0.52
1:B:158:ILE:CD1	1:B:172:VAL:HG21	2.40	0.52
1:B:346:THR:O	1:B:347:PHE:HB2	2.09	0.52
1:B:112:LEU:CD1	1:B:118:SER:HB2	2.39	0.52
1:A:420:LEU:O	1:A:424:ILE:HG13	2.09	0.51
1:A:144:LYS:O	1:A:147:ALA:HB3	2.11	0.51
1:B:298:PRO:O	1:B:302:MET:HG2	2.10	0.51
1:B:145:ASN:HA	1:B:148:ILE:HD12	1.92	0.51
1:A:372:TYR:O	1:A:375:TYR:HB3	2.11	0.51
1:A:276:GLU:CD	1:A:290:ASN:HD21	2.19	0.51
1:B:421:GLN:HA	1:B:421:GLN:OE1	2.10	0.51
1:B:172:VAL:HG11	1:B:178:LEU:HD12	1.92	0.50
1:B:286:PHE:CZ	1:B:288:GLU:HA	2.46	0.50
1:A:212:ILE:HD12	1:A:212:ILE:N	2.27	0.49
1:B:202:LYS:HG3	1:B:203:TYR:N	2.25	0.49
1:A:94:GLN:CG	1:A:97:ARG:NH1	2.76	0.49
1:B:346:THR:HB	1:B:348:LEU:HD22	1.95	0.49
1:B:181:SER:O	1:B:185:THR:OG1	2.26	0.49
1:B:158:ILE:HD12	1:B:172:VAL:HG23	1.95	0.49
1:B:158:ILE:HD12	1:B:172:VAL:CG2	2.43	0.48
1:B:55:PRO:HA	3:B:1434:HOH:O	2.12	0.47
1:B:4:LYS:O	1:B:76:VAL:HG22	2.14	0.47
1:B:252:LEU:HD22	1:B:284:PHE:HE1	1.80	0.47
1:B:427:ASP:OD1	1:B:443:LYS:HE3	2.14	0.47
1:A:356:ARG:HB2	3:A:1459:HOH:O	2.14	0.47
1:B:384:MET:HB2	3:B:1291:HOH:O	2.14	0.47
1:B:346:THR:OG1	1:B:348:LEU:HB2	2.14	0.47
1:B:442:LYS:HD2	1:B:442:LYS:C	2.40	0.47
1:B:156:VAL:HG11	1:B:200:MET:HE3	1.97	0.47
1:B:235:ARG:O	1:B:236:HIS:HB2	2.14	0.47
1:B:77:ALA:HB2	1:B:101:ILE:HB	1.97	0.47
1:B:133:GLY:HA2	1:B:152:ILE:CD1	2.45	0.47
1:B:149:ALA:HA	1:B:200:MET:CE	2.22	0.47
1:B:296:GLU:OE1	2:B:1001:PO4:O3	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:MET:HA	1:B:145:ASN:HB2	1.96	0.46
1:A:2:LEU:O	1:A:26:ILE:HG12	2.15	0.46
1:B:263:ALA:O	1:B:267:ILE:HG23	2.16	0.46
1:B:158:ILE:CD1	1:B:172:VAL:CG2	2.93	0.46
1:B:444:LEU:HB2	1:B:446:LEU:HD22	1.97	0.45
1:A:145:ASN:HA	1:A:148:ILE:HD12	1.98	0.45
1:A:123:MET:HB3	1:A:128:VAL:HB	1.99	0.45
1:B:23:GLU:OE1	1:B:310:LYS:NZ	2.38	0.45
1:B:278:LEU:HD23	1:B:278:LEU:HA	1.66	0.45
1:A:24:LEU:HA	1:A:24:LEU:HD23	1.65	0.45
1:A:154:TYR:HB3	1:A:155:PRO:HA	1.99	0.45
1:A:142:MET:HB3	1:A:146:ARG:NH2	2.32	0.45
1:B:5:ILE:O	1:B:5:ILE:HG13	2.11	0.45
1:A:235:ARG:N	1:A:441:GLU:OE1	2.46	0.45
1:B:324:LYS:C	1:B:327:GLU:HG3	2.42	0.45
1:B:35:ALA:HB2	1:B:54:ALA:HB2	1.99	0.44
1:B:251:GLU:OE2	1:B:251:GLU:N	2.41	0.44
1:A:427:ASP:OD2	1:A:429:ASN:N	2.51	0.44
1:B:199:TYR:C	1:B:199:TYR:CD1	2.93	0.44
1:B:427:ASP:OD2	1:B:429:ASN:N	2.51	0.44
1:B:212:ILE:HD13	1:B:227:GLU:CB	2.48	0.44
1:B:357:PHE:HA	1:B:410:ILE:O	2.18	0.44
1:A:404:ASN:ND2	3:A:1365:HOH:O	2.50	0.44
1:B:36:ASP:OD1	1:B:60:TYR:OH	2.31	0.44
1:B:297:HIS:CG	1:B:298:PRO:HD3	2.52	0.43
1:A:54:ALA:N	1:A:55:PRO:CD	2.81	0.43
1:A:141:ASP:OD2	1:A:143:ASP:HB2	2.17	0.43
1:B:152:ILE:CG2	1:B:202:LYS:HB2	2.48	0.43
1:A:207:PRO:O	1:A:436:ASN:HB2	2.19	0.43
1:B:79:HIS:ND1	1:B:80:PRO:HD2	2.33	0.43
1:A:94:GLN:HG3	1:A:97:ARG:HH22	1.78	0.43
1:B:133:GLY:C	1:B:152:ILE:HD11	2.44	0.43
1:B:172:VAL:HG11	1:B:178:LEU:CD1	2.49	0.43
1:A:116:LYS:O	1:A:120:ILE:HG12	2.18	0.43
1:B:241:GLU:OE2	1:B:336:GLU:OE1	2.36	0.43
1:A:209:HIS:CD2	1:A:209:HIS:C	2.96	0.43
1:B:63:ILE:HB	1:B:64:PRO:HD3	2.00	0.43
1:B:319:GLN:HA	1:B:320:PRO:HD3	1.90	0.42
1:A:89:ALA:O	1:A:93:GLU:HB2	2.19	0.42
1:A:104:GLY:HA2	3:A:1592:HOH:O	2.19	0.42
1:B:10:ARG:HD3	3:B:1346:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:CB	1:B:199:TYR:CE1	2.98	0.42
1:A:314:ARG:HB3	3:A:1314:HOH:O	2.19	0.42
1:B:199:TYR:C	1:B:199:TYR:HD1	2.27	0.42
1:B:28:THR:O	1:B:46:ASP:HB2	2.19	0.42
1:A:159:LYS:HB3	1:A:199:TYR:CZ	2.55	0.42
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.69	0.42
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.79	0.42
1:A:95:VAL:HG13	1:A:100:PHE:HB2	2.01	0.42
1:A:108:GLU:H	1:A:108:GLU:HG3	1.30	0.42
1:B:83:GLY:HA2	3:B:1370:HOH:O	2.19	0.42
1:B:356:ARG:NH2	1:B:412:ASP:OD1	2.44	0.42
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.76	0.42
1:A:212:ILE:HD13	1:A:277:PHE:CD1	2.55	0.42
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.61	0.42
1:A:5:ILE:HG23	1:A:26:ILE:HG21	2.02	0.41
1:A:323:ILE:H	1:A:323:ILE:HG12	1.55	0.41
1:B:90:ASN:O	1:B:94:GLN:HG3	2.20	0.41
1:B:343:ASP:O	1:B:347:PHE:N	2.51	0.41
1:B:446:LEU:N	1:B:446:LEU:CD1	2.83	0.41
1:A:62:ASN:ND2	1:A:65:ALA:HB2	2.35	0.41
1:B:144:LYS:O	1:B:147:ALA:HB3	2.21	0.41
1:B:287:ILE:HG21	1:B:287:ILE:HD13	1.85	0.41
1:A:327:GLU:C	1:A:329:HIS:CE1	2.99	0.41
3:A:1397:HOH:O	1:B:40:LYS:HE2	2.20	0.41
1:B:48:THR:C	1:B:49:VAL:HG23	2.46	0.41
1:A:119:ALA:O	1:A:123:MET:HG2	2.21	0.41
1:B:82:TYR:CD1	1:B:82:TYR:C	2.99	0.41
1:B:151:ARG:HD2	3:B:1411:HOH:O	2.19	0.41
1:A:235:ARG:HD2	1:A:446:LEU:HD23	2.03	0.41
1:B:19:ARG:HD2	3:B:1153:HOH:O	2.20	0.41
1:B:82:TYR:CZ	1:B:295:VAL:HG22	2.55	0.41
1:A:1:MET:SD	1:A:26:ILE:HD11	2.60	0.40
1:B:141:ASP:O	1:B:144:LYS:N	2.53	0.40
1:B:178:LEU:HD12	1:B:178:LEU:HA	1.90	0.40
1:B:244:PRO:HD2	1:B:333:HIS:ND1	2.36	0.40
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.85	0.40
1:A:357:PHE:HA	1:A:410:ILE:O	2.21	0.40
1:B:133:GLY:HA2	1:B:152:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/449 (96%)	418 (97%)	12 (3%)	0	100	100
1	B	424/449 (94%)	400 (94%)	23 (5%)	1 (0%)	43	36
All	All	854/898 (95%)	818 (96%)	35 (4%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	ASP

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	352/361 (98%)	329 (94%)	23 (6%)	15	8
1	B	338/361 (94%)	313 (93%)	25 (7%)	13	6
All	All	690/722 (96%)	642 (93%)	48 (7%)	14	7

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	37	ARG
1	A	40	LYS
1	A	56	SER
1	A	58	LYS

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Mol	Chain	Res	Type
1	A	72	ILE
1	A	108	GLU
1	A	140	ASP
1	A	142	MET
1	A	157	ILE
1	A	161	SER
1	A	169	MET
1	A	170	ARG
1	A	183	SER
1	A	185	THR
1	A	188[A]	GLU
1	A	188[B]	GLU
1	A	259	ARG
1	A	262	LYS
1	A	322	SER
1	A	323	ILE
1	A	326	GLU
1	A	442	LYS
1	B	1	MET
1	B	5	ILE
1	B	40	LYS
1	B	57	VAL
1	B	76	VAL
1	B	93	GLU
1	B	108	GLU
1	B	116	LYS
1	B	125	LYS
1	B	159	LYS
1	B	181	SER
1	B	182	ILE
1	B	199	TYR
1	B	202	LYS
1	B	204	LEU
1	B	234	ARG
1	B	237	GLN
1	B	323	ILE
1	B	327	GLU
1	B	348	LEU
1	B	353	LYS
1	B	382	ASP
1	B	393	GLU
1	B	446	LEU

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Mol	Chain	Res	Type
1	B	447	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	209	HIS
1	A	237	GLN
1	A	290	ASN
1	A	319	GLN
1	A	340	ASN
1	A	345	ASN
1	A	404	ASN
1	A	438	HIS
1	B	94	GLN
1	B	319	GLN
1	B	340	ASN
1	B	345	ASN
1	B	358	HIS
1	B	404	ASN
1	B	429	ASN
1	B	447	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	PO4	A	1000	-	4,4,4	2.47	3 (75%)	6,6,6	1.24	2 (33%)
2	PO4	B	1001	-	4,4,4	1.69	2 (50%)	6,6,6	1.01	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	PO4	P-O4	-2.92	1.46	1.54
2	A	1000	PO4	P-O3	-2.87	1.46	1.54
2	A	1000	PO4	P-O2	-2.76	1.46	1.54
2	B	1001	PO4	P-O2	-2.14	1.48	1.54
2	B	1001	PO4	P-O3	-2.05	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	PO4	O4-P-O2	2.09	114.40	107.91
2	A	1000	PO4	O2-P-O1	-2.00	103.88	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.