



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 02:38 PM EDT

PDB ID : 1DV1
Title : STRUCTURE OF BIOTIN CARBOXYLASE (APO)
Authors : Thoden, J.B.; Blanchard, C.Z.; Holden, H.M.; Waldrop, G.L.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

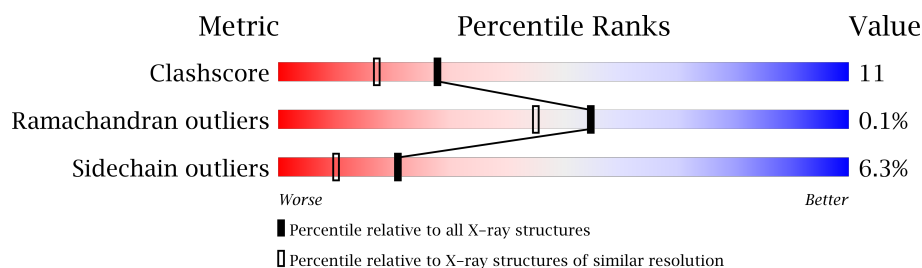
1 Overall quality at a glance

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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	
1	B	449	

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	2121	596	623	21			
1	B	428	Total	C	N	O	S	0	2	0
			3282	2077	582	605	18			

- Molecule 2 is PHOSPHATE ION (three-letter code: 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.

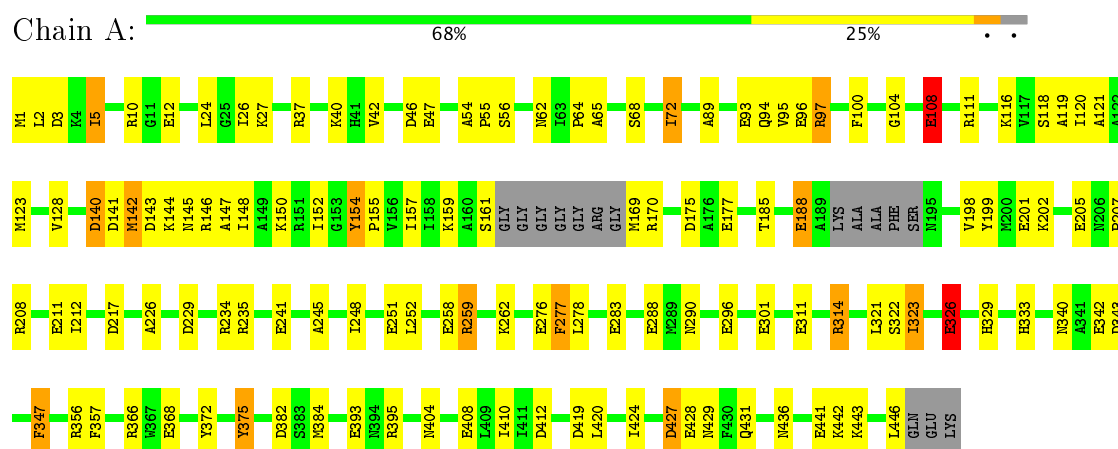
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	300	Total 300	O 300	0	0
3	B	244	Total 244	O 244	0	0

3 Residue-property plots

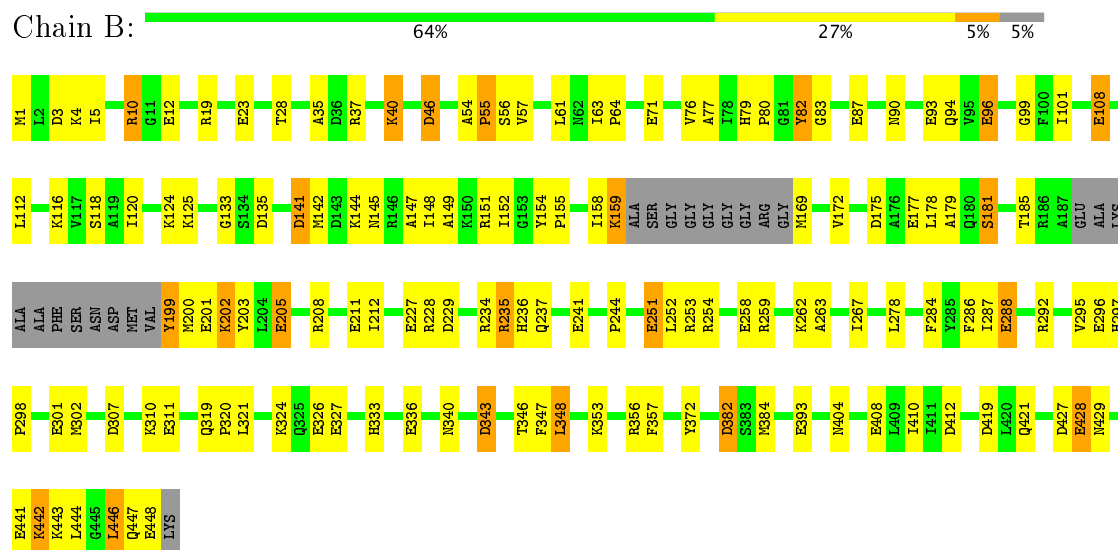
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: BIOTIN CARBOXYLASE



- Molecule 1: BIOTIN CARBOXYLASE



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	61.70 Å 95.80 Å 180.70 Å 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	1.06	24/3427 (0.7%)	1.38	32/4625 (0.7%)
1	B	1.04	19/3351 (0.6%)	1.35	24/4532 (0.5%)
All	All	1.05	43/6778 (0.6%)	1.36	56/9157 (0.6%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CD-OE2	12.26	1.39	1.25
1	B	326	GLU	CD-OE2	8.44	1.34	1.25
1	A	251	GLU	CD-OE2	8.25	1.34	1.25
1	B	288	GLU	CD-OE2	8.04	1.34	1.25
1	A	368	GLU	CD-OE2	7.55	1.33	1.25
1	B	96	GLU	CD-OE2	7.26	1.33	1.25
1	A	288	GLU	CD-OE2	6.79	1.33	1.25
1	A	326	GLU	CD-OE2	6.77	1.33	1.25
1	B	251	GLU	CD-OE2	6.73	1.33	1.25
1	A	342	GLU	CD-OE2	6.56	1.32	1.25
1	B	87	GLU	CD-OE2	6.53	1.32	1.25
1	B	428	GLU	CD-OE2	6.52	1.32	1.25
1	A	47	GLU	CD-OE2	6.51	1.32	1.25
1	B	205	GLU	CD-OE2	6.46	1.32	1.25
1	B	71	GLU	CD-OE2	6.44	1.32	1.25
1	B	448	GLU	CD-OE2	6.44	1.32	1.25
1	B	108	GLU	CD-OE2	6.43	1.32	1.25
1	A	258	GLU	CD-OE2	6.36	1.32	1.25
1	B	441	GLU	CD-OE2	6.34	1.32	1.25
1	A	12	GLU	CD-OE2	6.25	1.32	1.25
1	A	96	GLU	CD-OE2	6.19	1.32	1.25
1	A	241	GLU	CD-OE2	6.18	1.32	1.25
1	A	177	GLU	CD-OE2	6.17	1.32	1.25
1	B	93	GLU	CD-OE2	6.16	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CD-OE2	6.14	1.32	1.25
1	A	393	GLU	CD-OE2	5.89	1.32	1.25
1	B	12	GLU	CD-OE2	5.88	1.32	1.25
1	B	408	GLU	CD-OE2	5.87	1.32	1.25
1	A	201	GLU	CD-OE2	5.83	1.32	1.25
1	B	311	GLU	CD-OE2	5.83	1.32	1.25
1	B	301	GLU	CD-OE2	5.70	1.31	1.25
1	A	296	GLU	CD-OE1	-5.69	1.19	1.25
1	A	408	GLU	CD-OE1	-5.65	1.19	1.25
1	A	301	GLU	CD-OE2	5.63	1.31	1.25
1	B	258	GLU	CD-OE2	5.47	1.31	1.25
1	A	188[A]	GLU	CD-OE2	5.34	1.31	1.25
1	A	188[B]	GLU	CD-OE2	5.34	1.31	1.25
1	A	283	GLU	CD-OE2	5.33	1.31	1.25
1	B	211	GLU	CD-OE1	-5.23	1.19	1.25
1	A	428	GLU	CD-OE2	5.21	1.31	1.25
1	A	211	GLU	CD-OE2	5.18	1.31	1.25
1	B	201	GLU	CD-OE2	5.05	1.31	1.25
1	A	311	GLU	CD-OE2	5.05	1.31	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	A	10	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	A	366	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	111	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	314	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	A	366	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	3	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	B	3	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	253	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	229	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	375	TYR	CB-CG-CD1	-7.33	116.60	121.00
1	B	254	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	395	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	229	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	3	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	343	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	259	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	175	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	419[A]	ASP	CB-CG-OD1	6.56	124.21	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419[B]	ASP	CB-CG-OD1	6.56	124.21	118.30
1	A	419[A]	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	419[B]	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	10	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	228	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	175	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	372	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	382	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	175	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	140	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	42	VAL	CA-CB-CG1	-5.90	102.05	110.90
1	A	234	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	395	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	217	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	208	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	427	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	B	46	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	292	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	154	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	382	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	329	HIS	CA-CB-CG	-5.48	104.28	113.60
1	B	307	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	82	TYR	N-CA-CB	5.37	120.27	110.60
1	A	46	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	343	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	277	PHE	CB-CA-C	-5.27	99.87	110.40
1	A	259	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	226	ALA	CB-CA-C	5.25	117.97	110.10
1	B	228	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	208	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	347	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	B	419	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	375	TYR	CB-CG-CD2	5.15	124.09	121.00
1	B	55	PRO	N-CA-CB	5.11	109.43	103.30
1	B	135[A]	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	135[B]	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	3	ASP	CB-CG-OD1	5.05	122.84	118.30

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	3372	59	0
1	B	3282	0	3264	90	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	300	0	0	9	0
3	B	244	0	0	9	0
All	All	7197	0	6636	149	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 11.

All (149) 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:235:ARG:HH12	1:B:446:LEU:HB3	1.22	1.01
1:B:152:ILE:HD12	1:B:200:MET:HE2	1.41	0.98
1:B:149:ALA:HA	1:B:200:MET:HE3	1.55	0.88
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:HA	1:B:200:MET:CE	2.22	0.70
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:179:ALA:HB3	3:B:1532:HOH:O	2.09	0.52
1:B:96:GLU:O	1:B:99:GLY:N	2.35	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:B:421:GLN:HA	1:B:421:GLN:OE1	2.10	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:THR:HB	1:B:348:LEU:HD22	1.95	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:235:ARG:O	1:B:236:HIS:HB2	2.14	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:77:ALA:HB2	1:B:101:ILE:HB	1.97	0.47
1:B:296:GLU:OE1	2:B:1001:PO4:O3	2.33	0.47
1:B:133:GLY:HA2	1:B:152:ILE:CD1	2.45	0.47
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:A:276:GLU:CD	1:A:290:ASN:HD21	2.19	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:278:LEU:HD23	1:B:278:LEU:HA	1.66	0.45
1:A:154:TYR:HB3	1:A:155:PRO:HA	1.99	0.45
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.65	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: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: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:23:GLU:OE1	1:B:310:LYS:NZ	2.38	0.44
1:B:297:HIS:CG	1:B:298:PRO:HD3	2.52	0.43
1:A:141:ASP:OD2	1:A:143:ASP:HB2	2.17	0.43
1:A:54:ALA:N	1:A:55:PRO:CD	2.81	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:104:GLY:HA2	3:A:1592:HOH:O	2.19	0.42
1:A:89:ALA:O	1:A:93:GLU:HB2	2.19	0.42
1:B:10:ARG:HD3	3:B:1346:HOH:O	2.19	0.42
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: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:HA	1:B:444:LEU:HD23	1.79	0.42
1:A:95:VAL:HG13	1:A:100:PHE:HB2	2.01	0.42
1:A:108:GLU:HG3	1:A:108:GLU:H	1.30	0.42
1:B:356:ARG:NH2	1:B:412:ASP:OD1	2.44	0.42
1:B:442:LYS:HD2	1:B:442:LYS:C	2.40	0.42
1:B:83:GLY:HA2	3:B:1370:HOH:O	2.19	0.42
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.76	0.42
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.61	0.42
1:A:212:ILE:HD13	1:A:277:PHE:CD1	2.55	0.42
1:A:323:ILE:H	1:A:323:ILE:HG12	1.55	0.41
1:A:5:ILE:HG23	1:A:26:ILE:HG21	2.02	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:199:TYR:C	1:B:199:TYR:CD1	2.93	0.41
1:B:446:LEU:CD1	1:B:446:LEU:N	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:HD13	1:B:287:ILE:HG21	1.85	0.41
3:A:1397:HOH:O	1:B:40:LYS:HE2	2.20	0.41
1:A:119:ALA:O	1:A:123:MET:HG2	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HA	1:B:178:LEU:HD12	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%)	51	41
All	All	854/898 (95%)	818 (96%)	35 (4%)	1 (0%)	55	45

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/361 (98%)	331 (94%)	21 (6%)	22	11
1	B	338/361 (94%)	315 (93%)	23 (7%)	18	8
All	All	690/722 (96%)	646 (94%)	44 (6%)	21	10

All (44) 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	72	ILE
1	A	97	ARG
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	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	10	ARG
1	B	37	ARG
1	B	40	LYS
1	B	57	VAL
1	B	108	GLU
1	B	116	LYS
1	B	125	LYS
1	B	159	LYS
1	B	181	SER
1	B	199	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	202	LYS
1	B	234	ARG
1	B	235	ARG
1	B	237	GLN
1	B	262	LYS
1	B	348	LEU
1	B	353	LYS
1	B	382	ASP
1	B	393	GLU
1	B	442	LYS
1	B	446	LEU
1	B	447	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	404	ASN
1	B	94	GLN
1	B	319	GLN
1	B	340	ASN
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 carbohydrates 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	1.98	3 (75%)	6,6,6	1.04	0
2	PO4	B	1001	-	4,4,4	1.34	0	6,6,6	0.85	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
2	PO4	A	1000	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1001	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	PO4	P-O4	-2.34	1.46	1.54
2	A	1000	PO4	P-O3	-2.29	1.46	1.54
2	A	1000	PO4	P-O2	-2.20	1.46	1.54

There are no bond angle outliers.

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 [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.