



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:02 PM GMT

PDB ID : 1BNC
Title : THREE-DIMENSIONAL STRUCTURE OF THE BIOTIN CARBOXYLASE
SUBUNIT OF ACETYL-COA CARBOXYLASE
Authors : Waldrop, G.; Rayment, I.; Holden, H.M.
Deposited on : 1994-07-06
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

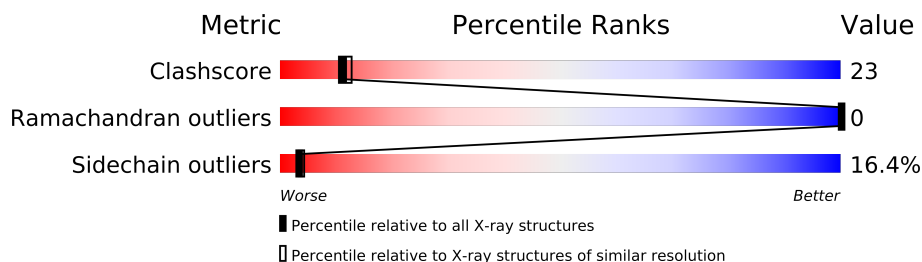
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 6743 atoms, of which 0 are hydrogen and 0 are deuterium.

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	433	Total	C	N	O	S	0	0	0
			3356	2119	599	617	21			
1	B	424	Total	C	N	O	S	0	0	0
			3261	2059	580	603	19			

- 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.

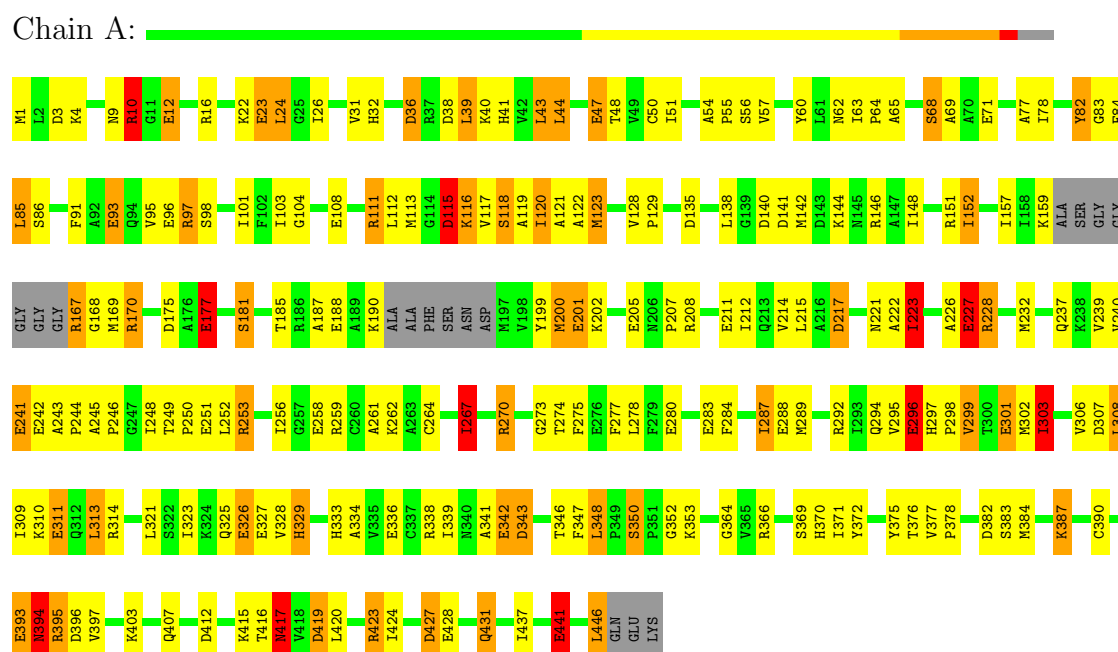
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0
3	B	50	Total 50	O 50	0	0

3 Residue-property plots

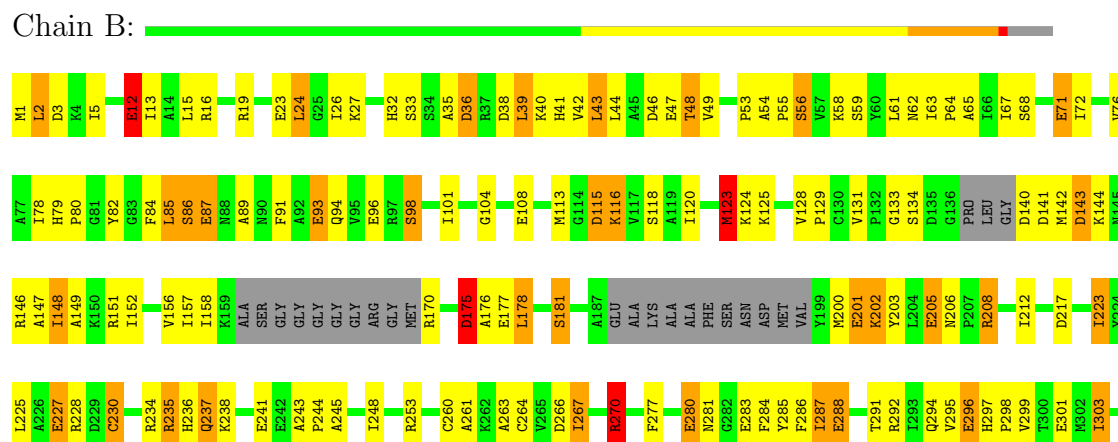
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

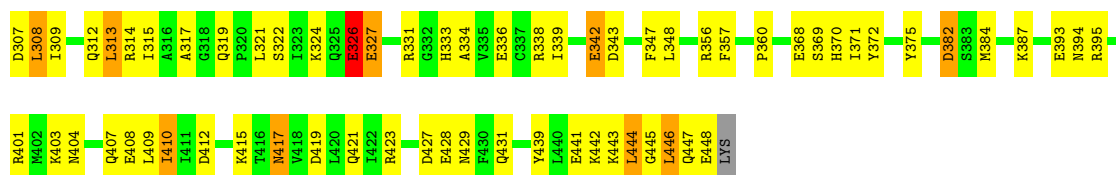
Note EDS was not executed.

• Molecule 1: BIOTIN CARBOXYLASE



• Molecule 1: BIOTIN CARBOXYLASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.90Å 96.10Å 180.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6743	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: 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	1.08	29/3416 (0.8%)	1.41	48/4609 (1.0%)
1	B	1.05	24/3318 (0.7%)	1.35	33/4480 (0.7%)
All	All	1.06	53/6734 (0.8%)	1.38	81/9089 (0.9%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLU	CD-OE2	-8.70	1.16	1.25
1	A	47	GLU	CD-OE1	8.29	1.34	1.25
1	A	205	GLU	CD-OE1	7.98	1.34	1.25
1	A	188	GLU	CD-OE2	7.72	1.34	1.25
1	A	311	GLU	CD-OE1	7.66	1.34	1.25
1	A	280	GLU	CD-OE2	7.13	1.33	1.25
1	B	296	GLU	CD-OE2	7.08	1.33	1.25
1	B	448	GLU	CD-OE1	6.95	1.33	1.25
1	B	326	GLU	CD-OE2	6.84	1.33	1.25
1	B	87	GLU	CD-OE1	6.76	1.33	1.25
1	A	288	GLU	CD-OE2	6.74	1.33	1.25
1	B	205	GLU	CD-OE1	6.70	1.33	1.25
1	A	241	GLU	CD-OE1	6.69	1.33	1.25
1	A	227	GLU	CD-OE2	-6.64	1.18	1.25
1	A	12	GLU	CD-OE1	6.60	1.32	1.25
1	A	108	GLU	CD-OE2	6.56	1.32	1.25
1	A	201	GLU	CD-OE1	6.54	1.32	1.25
1	A	428	GLU	CD-OE1	6.53	1.32	1.25
1	B	108	GLU	CD-OE1	6.52	1.32	1.25
1	A	301	GLU	CD-OE1	6.39	1.32	1.25
1	B	327	GLU	CD-OE1	6.38	1.32	1.25
1	A	441	GLU	CD-OE1	6.37	1.32	1.25
1	B	93	GLU	CD-OE1	6.33	1.32	1.25
1	A	258	GLU	CD-OE1	6.28	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	GLU	CD-OE1	6.25	1.32	1.25
1	A	242	GLU	CD-OE1	6.25	1.32	1.25
1	A	283	GLU	CD-OE2	6.24	1.32	1.25
1	B	283	GLU	CD-OE2	6.23	1.32	1.25
1	A	71	GLU	CD-OE1	6.15	1.32	1.25
1	B	71	GLU	CD-OE2	6.05	1.32	1.25
1	B	96	GLU	CD-OE1	5.93	1.32	1.25
1	B	342	GLU	CD-OE1	5.90	1.32	1.25
1	B	441	GLU	CD-OE1	5.83	1.32	1.25
1	B	23	GLU	CD-OE2	5.83	1.32	1.25
1	B	47	GLU	CD-OE1	5.81	1.32	1.25
1	A	96	GLU	CD-OE1	5.80	1.32	1.25
1	A	251	GLU	CD-OE1	5.75	1.31	1.25
1	B	280	GLU	CD-OE2	5.75	1.31	1.25
1	B	428	GLU	CD-OE1	5.66	1.31	1.25
1	A	227	GLU	CD-OE1	5.66	1.31	1.25
1	B	288	GLU	CD-OE2	5.61	1.31	1.25
1	B	12	GLU	CD-OE1	5.60	1.31	1.25
1	A	93	GLU	CD-OE1	5.55	1.31	1.25
1	A	393	GLU	CD-OE1	5.55	1.31	1.25
1	B	393	GLU	CD-OE1	5.46	1.31	1.25
1	B	408	GLU	CD-OE2	5.41	1.31	1.25
1	A	327	GLU	CD-OE2	5.39	1.31	1.25
1	A	326	GLU	CD-OE1	5.38	1.31	1.25
1	A	177	GLU	CD-OE1	5.36	1.31	1.25
1	A	342	GLU	CD-OE2	5.20	1.31	1.25
1	B	201	GLU	CD-OE2	5.20	1.31	1.25
1	A	23	GLU	CD-OE2	5.19	1.31	1.25
1	B	301	GLU	CD-OE1	5.13	1.31	1.25

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	A	417	ASN	N-CA-CB	-9.33	93.81	110.60
1	B	228	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	270	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	175	ASP	CB-CG-OD1	7.92	125.42	118.30
1	B	382	ASP	CB-CG-OD1	-7.76	111.31	118.30
1	A	419	ASP	CB-CG-OD1	-7.75	111.32	118.30
1	B	417	ASN	N-CA-CB	-7.49	97.12	110.60
1	B	419	ASP	CB-CG-OD1	-7.47	111.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	ASP	CB-CG-OD1	-7.43	111.62	118.30
1	A	140	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	A	175	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	B	394	ASN	CB-CA-C	-7.07	96.27	110.40
1	A	259	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	3	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	B	143	ASP	CB-CG-OD1	-6.86	112.12	118.30
1	B	46	ASP	CB-CG-OD1	-6.86	112.13	118.30
1	A	423	ARG	N-CA-CB	-6.80	98.36	110.60
1	B	3	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	B	175	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	B	208	ARG	N-CA-CB	6.68	122.62	110.60
1	A	38	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	A	111	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	123	MET	CG-SD-CE	6.50	110.60	100.20
1	B	253	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	287	ILE	CB-CA-C	-6.38	98.84	111.60
1	B	38	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	A	135	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	B	36	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	A	135	ASP	CB-CG-OD2	6.16	123.85	118.30
1	B	417	ASN	CB-CA-C	-6.15	98.11	110.40
1	A	38	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	115	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	A	36	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	B	123	MET	CA-CB-CG	-6.08	102.97	113.30
1	A	228	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	266	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	382	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	423	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	217	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	B	3	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	253	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	226	ALA	N-CA-CB	5.87	118.32	110.10
1	A	303	ILE	CA-CB-CG2	5.84	122.59	110.90
1	A	253	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	140	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	10	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	140	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	287	ILE	CB-CA-C	-5.78	100.04	111.60
1	A	314	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	395	ARG	NE-CZ-NH2	-5.68	117.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	259	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	223	ILE	CA-CB-CG2	5.62	122.15	110.90
1	B	423	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	83	GLY	C-N-CA	-5.49	107.97	121.70
1	B	419	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	38	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	175	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	419	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	329	HIS	CA-CB-CG	-5.35	104.51	113.60
1	A	396	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	412	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	267	ILE	N-CA-CB	-5.29	98.64	110.80
1	A	314	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	111	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	401	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	217	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	3	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	343	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	141	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	343	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	395	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	115	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	395	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	115	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	427	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	394	ASN	N-CA-CB	5.12	119.82	110.60
1	B	141	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	141	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	366	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3356	0	3391	138	0
1	B	3261	0	3260	163	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
3	A	66	0	0	1	0
3	B	50	0	0	5	0
All	All	6743	0	6651	300	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (300) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:ILE:HD11	1:A:201:GLU:HB3	1.42	1.00
1:B:244:PRO:HD2	1:B:333:HIS:CD2	2.05	0.91
1:B:203:TYR:HE2	1:B:205:GLU:HG3	1.35	0.90
1:A:264:CYS:O	1:A:267:ILE:HG22	1.74	0.88
1:B:36:ASP:HB3	1:B:39:LEU:HD22	1.55	0.87
1:A:296:GLU:OE2	2:A:953:PO4:O3	1.92	0.87
1:A:256:ILE:HD12	1:A:284:PHE:CG	2.11	0.86
1:A:157:ILE:CD1	1:A:201:GLU:HB3	2.06	0.85
1:B:113:MET:HE2	1:B:267:ILE:HD12	1.59	0.85
1:A:31:VAL:HB	1:A:51:ILE:HD13	1.59	0.83
1:B:113:MET:CE	1:B:267:ILE:HD12	2.08	0.82
1:A:54:ALA:HB3	1:A:55:PRO:HD3	1.63	0.81
1:B:203:TYR:CE2	1:B:205:GLU:HG3	2.14	0.81
1:B:175:ASP:O	1:B:178:LEU:HB2	1.83	0.78
1:A:112:LEU:HD12	1:A:118:SER:HB2	1.66	0.78
1:B:148:ILE:HG23	1:B:149:ALA:H	1.49	0.78
1:B:1:MET:CE	1:B:313:LEU:HB3	2.15	0.77
1:B:263:ALA:O	1:B:267:ILE:HG23	1.84	0.77
1:A:427:ASP:O	1:A:431:GLN:HG3	1.85	0.77
1:B:303:ILE:HD11	1:B:334:ALA:N	1.99	0.76
1:B:1:MET:HE1	1:B:313:LEU:HB3	1.68	0.75
1:A:112:LEU:CD1	1:A:118:SER:HB2	2.18	0.74
1:B:202:LYS:HG3	1:B:203:TYR:N	2.03	0.72
1:B:212:ILE:HD13	1:B:227:GLU:HB3	1.71	0.71
1:B:296:GLU:OE1	2:B:954:PO4:O3	2.09	0.71
1:B:157:ILE:HG13	1:B:170:ARG:O	1.91	0.70
1:A:123:MET:CE	1:A:128:VAL:HG21	2.20	0.70
1:B:134:SER:HA	1:B:148:ILE:HD11	1.71	0.70
1:A:261:ALA:O	1:A:264:CYS:HB2	1.90	0.70
1:B:115:ASP:HB3	1:B:118:SER:OG	1.90	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:104:GLY:O	1:A:270:ARG:NH1	2.24	0.69
1:A:144:LYS:O	1:A:148:ILE:HG13	1.94	0.68
1:B:120:ILE:HG22	1:B:124:LYS:HD2	1.76	0.68
1:A:91:PHE:O	1:A:95:VAL:HG23	1.94	0.68
1:B:55:PRO:HG2	1:B:58:LYS:HG3	1.75	0.67
1:A:339:ILE:HA	1:A:417:ASN:ND2	2.10	0.66
1:A:159:LYS:N	1:A:199:TYR:O	2.27	0.66
1:A:207:PRO:O	1:A:437:ILE:HG12	1.95	0.65
1:A:341:ALA:O	1:A:383:SER:HB2	1.97	0.65
1:B:1:MET:SD	1:B:317:ALA:HB2	2.36	0.65
1:A:170:ARG:NH1	1:A:181:SER:OG	2.29	0.65
1:A:227:GLU:OE2	1:A:253:ARG:NE	2.26	0.65
1:B:427:ASP:O	1:B:431:GLN:HG3	1.96	0.65
1:B:63:ILE:HB	1:B:64:PRO:HD3	1.79	0.65
1:A:256:ILE:HD12	1:A:284:PHE:CD2	2.32	0.64
1:A:394:ASN:OD1	1:A:397:VAL:HG23	1.97	0.64
1:B:356:ARG:HB3	1:B:412:ASP:HB2	1.80	0.64
1:B:148:ILE:HG23	1:B:149:ALA:N	2.11	0.64
1:B:120:ILE:HG22	1:B:124:LYS:CD	2.27	0.64
1:B:123:MET:CG	1:B:128:VAL:HB	2.28	0.64
1:B:324:LYS:O	1:B:327:GLU:HB2	1.99	0.63
1:A:120:ILE:O	1:A:123:MET:HB2	1.99	0.62
1:A:23:GLU:OE1	1:A:310:LYS:NZ	2.28	0.62
1:A:116:LYS:O	1:A:120:ILE:HD12	1.99	0.62
1:A:303:ILE:HD11	1:A:334:ALA:N	2.14	0.62
1:B:427:ASP:OD1	1:B:429:ASN:HB2	2.00	0.62
1:A:297:HIS:HB2	1:A:308:LEU:HD23	1.82	0.61
1:B:427:ASP:OD2	1:B:443:LYS:HE3	2.00	0.60
1:B:156:VAL:HG12	1:B:157:ILE:N	2.15	0.60
1:A:181:SER:O	1:A:185:THR:HG23	2.01	0.60
1:A:343:ASP:O	1:A:347:PHE:N	2.31	0.60
1:A:420:LEU:O	1:A:424:ILE:HG13	2.02	0.60
1:B:36:ASP:CB	1:B:39:LEU:HD22	2.30	0.60
1:B:116:LYS:O	1:B:120:ILE:HG13	2.01	0.60
1:B:123:MET:HG3	1:B:128:VAL:HB	1.83	0.60
1:B:16:ARG:CG	1:B:309:ILE:HD13	2.33	0.59
1:A:56:SER:HG	1:A:84:PHE:HE1	1.47	0.59
1:B:16:ARG:NE	1:B:309:ILE:CD1	2.64	0.59
1:B:158:ILE:N	1:B:158:ILE:HD13	2.17	0.59
1:A:275:PHE:CE1	1:A:289:MET:HE3	2.38	0.58
1:B:369:SER:OG	1:B:371:ILE:HG12	2.04	0.58
1:B:343:ASP:O	1:B:347:PHE:N	2.28	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:156:VAL:HG11	1:B:200:MET:CG	2.34	0.58
1:A:369:SER:OG	1:A:371:ILE:HG12	2.04	0.57
1:B:286:PHE:CZ	1:B:288:GLU:HA	2.39	0.57
1:A:217:ASP:OD2	1:A:221:ASN:ND2	2.23	0.57
1:B:104:GLY:O	1:B:270:ARG:NH1	2.37	0.57
1:B:175:ASP:N	1:B:175:ASP:OD1	2.32	0.56
1:A:63:ILE:N	1:A:64:PRO:HD2	2.19	0.56
1:B:295:VAL:HG23	2:B:954:PO4:O4	2.05	0.56
1:B:421:GLN:HA	1:B:421:GLN:OE1	2.06	0.56
1:A:339:ILE:HA	1:A:417:ASN:HD21	1.70	0.56
1:B:241:GLU:HG2	1:B:296:GLU:HG2	1.88	0.56
1:B:384:MET:HE1	1:B:387:LYS:HG2	1.88	0.56
1:A:32:HIS:O	1:A:50:CYS:HA	2.06	0.56
1:B:1:MET:HE2	1:B:313:LEU:HB3	1.88	0.56
1:B:245:ALA:HB3	1:B:248:ILE:HG13	1.86	0.56
1:B:410:ILE:HG22	1:B:410:ILE:O	2.05	0.56
1:B:120:ILE:CG2	1:B:124:LYS:HD2	2.35	0.56
1:B:303:ILE:HD11	1:B:333:HIS:C	2.26	0.55
1:A:128:VAL:HG13	1:A:129:PRO:HD2	1.89	0.55
1:B:148:ILE:O	1:B:151:ARG:HB3	2.06	0.55
1:A:63:ILE:HB	1:A:64:PRO:HD3	1.88	0.55
1:B:241:GLU:OE1	1:B:336:GLU:OE2	2.25	0.55
1:A:376:THR:O	1:A:378:PRO:HD3	2.07	0.55
1:A:301:GLU:HG2	1:A:306:VAL:O	2.07	0.55
1:B:294:GLN:HB3	1:B:296:GLU:OE1	2.07	0.55
1:B:309:ILE:O	1:B:312:GLN:HB2	2.08	0.54
1:B:404:ASN:HB2	3:B:987:HOH:O	2.07	0.54
1:A:115:ASP:OD2	1:A:118:SER:OG	2.26	0.54
1:A:303:ILE:HD11	1:A:333:HIS:CA	2.37	0.54
1:A:303:ILE:HD11	1:A:333:HIS:HA	1.88	0.54
1:A:343:ASP:N	1:A:348:LEU:O	2.37	0.54
1:B:357:PHE:HA	1:B:410:ILE:O	2.08	0.54
1:B:149:ALA:N	1:B:200:MET:HE1	2.22	0.54
1:B:2:LEU:O	1:B:26:ILE:HG12	2.07	0.54
1:B:68:SER:O	1:B:71:GLU:HB2	2.08	0.54
1:B:303:ILE:HD12	1:B:334:ALA:CB	2.38	0.54
1:B:149:ALA:CA	1:B:200:MET:HE1	2.38	0.54
1:B:149:ALA:HA	1:B:200:MET:CE	2.37	0.54
1:A:39:LEU:HD23	1:A:41:HIS:HE1	1.73	0.54
1:B:442:LYS:O	1:B:445:GLY:N	2.40	0.54
1:A:4:LYS:NZ	1:A:47:GLU:OE2	2.41	0.54
1:B:331:ARG:NH2	3:B:1002:HOH:O	2.40	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:177:GLU:O	1:B:181:SER:HB2	2.08	0.53
1:A:228:ARG:CD	1:A:299:VAL:HG12	2.37	0.53
1:B:202:LYS:HG3	1:B:203:TYR:H	1.72	0.53
1:B:261:ALA:O	1:B:264:CYS:HB2	2.08	0.53
1:A:298:PRO:O	1:A:302:MET:HG2	2.09	0.53
1:A:115:ASP:OD1	1:A:117:VAL:HB	2.08	0.53
1:B:85:LEU:HB3	1:B:91:PHE:CD2	2.44	0.53
1:B:384:MET:HE2	1:B:387:LYS:HG3	1.91	0.53
1:A:241:GLU:OE1	1:A:336:GLU:OE2	2.27	0.53
1:A:123:MET:HE3	1:A:128:VAL:CG2	2.39	0.53
1:B:16:ARG:HG3	1:B:309:ILE:HD13	1.90	0.53
1:B:235:ARG:O	1:B:236:HIS:HB2	2.09	0.53
1:A:113:MET:HE2	1:A:119:ALA:HA	1.91	0.53
1:A:297:HIS:CG	1:A:298:PRO:HD3	2.44	0.52
1:A:350:SER:OG	1:A:350:SER:O	2.28	0.52
1:A:63:ILE:HG23	1:A:91:PHE:HD1	1.74	0.52
1:A:342:GLU:HA	1:A:348:LEU:O	2.10	0.52
1:A:93:GLU:CD	1:A:111:ARG:HH22	2.13	0.52
1:B:1:MET:HE3	1:B:26:ILE:CD1	2.40	0.52
1:A:211:GLU:HG3	1:A:274:THR:HG21	1.91	0.52
1:B:113:MET:HE3	1:B:267:ILE:HD12	1.90	0.52
1:B:370:HIS:ND1	1:B:370:HIS:N	2.46	0.52
1:A:275:PHE:CZ	1:A:289:MET:HE1	2.45	0.51
1:A:441:GLU:HG2	1:A:446:LEU:HB3	1.92	0.51
1:B:134:SER:HA	1:B:148:ILE:CD1	2.39	0.51
1:A:36:ASP:HB3	1:A:39:LEU:HD22	1.91	0.51
1:A:138:LEU:HD21	1:A:200:MET:CE	2.41	0.51
1:B:79:HIS:ND1	1:B:80:PRO:HD2	2.26	0.51
1:A:275:PHE:CZ	1:A:289:MET:CE	2.94	0.50
1:B:384:MET:CE	1:B:387:LYS:HG2	2.41	0.50
1:B:12:GLU:HB3	3:B:980:HOH:O	2.11	0.50
1:B:360:PRO:HD3	1:B:409:LEU:HD13	1.92	0.50
1:B:63:ILE:CB	1:B:64:PRO:HD3	2.42	0.50
1:A:120:ILE:HG22	1:A:121:ALA:N	2.26	0.50
1:B:16:ARG:HD3	3:B:981:HOH:O	2.12	0.50
1:B:1:MET:HE3	1:B:26:ILE:HD11	1.93	0.49
1:A:245:ALA:HB3	1:A:248:ILE:HG13	1.92	0.49
1:A:303:ILE:HD11	1:A:333:HIS:C	2.32	0.49
1:B:16:ARG:NE	1:B:309:ILE:HD13	2.26	0.49
1:A:228:ARG:HD3	1:A:299:VAL:HG12	1.93	0.49
1:A:214:VAL:HG22	1:A:273:GLY:O	2.13	0.49
1:B:427:ASP:OD2	1:B:439:TYR:OH	2.29	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:ILE:HG12	1:A:325:GLN:OE1	2.12	0.49
1:A:187:ALA:O	1:A:190:LYS:O	2.30	0.49
1:A:148:ILE:O	1:A:151:ARG:HB3	2.13	0.48
1:A:63:ILE:N	1:A:64:PRO:CD	2.76	0.48
1:B:144:LYS:O	1:B:147:ALA:N	2.45	0.48
1:B:303:ILE:HD12	1:B:334:ALA:HB3	1.95	0.48
1:A:123:MET:HE3	1:A:128:VAL:HG21	1.94	0.48
1:B:43:LEU:CD1	1:B:43:LEU:N	2.77	0.48
1:B:149:ALA:HA	1:B:200:MET:HE3	1.94	0.48
1:B:444:LEU:HB3	1:B:446:LEU:HD13	1.95	0.48
1:A:24:LEU:HB3	1:A:26:ILE:HG13	1.96	0.48
1:B:175:ASP:HA	1:B:178:LEU:HD22	1.95	0.48
1:B:32:HIS:HD2	1:B:33:SER:O	1.96	0.48
1:A:338:ARG:HD3	1:A:384:MET:CE	2.44	0.48
1:B:78:ILE:O	1:B:80:PRO:HD3	2.14	0.48
1:A:249:THR:HB	1:A:250:PRO:HD2	1.95	0.48
1:B:131:VAL:HG22	1:B:285:TYR:HB3	1.95	0.48
1:B:372:TYR:O	1:B:375:TYR:HB3	2.14	0.47
1:A:215:LEU:O	1:A:222:ALA:HA	2.13	0.47
1:B:291:THR:O	1:B:292:ARG:HB3	2.15	0.47
1:A:56:SER:OG	1:A:84:PHE:HE1	1.97	0.47
1:B:53:PRO:C	1:B:55:PRO:HD2	2.35	0.47
1:B:427:ASP:OD1	1:B:429:ASN:N	2.47	0.47
1:A:211:GLU:HG3	1:A:274:THR:CG2	2.45	0.47
1:A:39:LEU:HD23	1:A:41:HIS:CE1	2.49	0.47
1:A:62:ASN:ND2	1:A:65:ALA:HB2	2.29	0.47
1:B:89:ALA:O	1:B:93:GLU:HB2	2.14	0.47
1:B:15:LEU:O	1:B:19:ARG:HG3	2.15	0.47
1:B:1:MET:CE	1:B:26:ILE:HD11	2.45	0.47
1:B:16:ARG:NH2	1:B:307:ASP:OD1	2.46	0.46
1:B:297:HIS:N	1:B:298:PRO:CD	2.78	0.46
1:B:384:MET:HE2	1:B:387:LYS:CG	2.46	0.46
1:B:56:SER:HA	1:B:59:SER:OG	2.16	0.46
1:A:372:TYR:O	1:A:375:TYR:HB3	2.15	0.46
1:B:339:ILE:HA	1:B:417:ASN:HD22	1.80	0.46
1:A:297:HIS:N	1:A:298:PRO:CD	2.79	0.46
1:A:267:ILE:HD13	1:A:267:ILE:HG21	1.29	0.46
1:A:275:PHE:CE1	1:A:289:MET:CE	2.99	0.46
1:B:158:ILE:N	1:B:158:ILE:CD1	2.77	0.46
1:B:16:ARG:NE	1:B:309:ILE:HD12	2.30	0.45
1:A:54:ALA:HB3	1:A:55:PRO:CD	2.40	0.45
1:A:441:GLU:HG2	1:A:446:LEU:CB	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:LEU:O	1:A:423:ARG:HB3	2.16	0.45
1:B:94:GLN:O	1:B:98:SER:OG	2.29	0.45
1:B:1:MET:HE3	1:B:2:LEU:HD12	1.98	0.45
1:B:241:GLU:OE2	1:B:338:ARG:NE	2.36	0.45
1:A:39:LEU:HA	1:A:39:LEU:HD12	1.60	0.45
1:A:113:MET:HE1	1:A:122:ALA:HB3	1.97	0.45
1:B:101:ILE:O	1:B:101:ILE:HG22	2.12	0.45
1:B:303:ILE:CD1	1:B:334:ALA:CB	2.95	0.45
1:B:54:ALA:N	1:B:55:PRO:CD	2.79	0.45
1:A:306:VAL:HG12	1:A:307:ASP:N	2.32	0.45
1:A:370:HIS:N	1:A:370:HIS:ND1	2.61	0.45
1:A:364:GLY:O	1:A:390:CYS:HA	2.17	0.45
1:B:87:GLU:HG2	1:B:291:THR:OG1	2.16	0.44
1:A:241:GLU:CD	1:A:296:GLU:HG2	2.37	0.44
1:A:85:LEU:HB3	1:A:91:PHE:CD2	2.52	0.44
1:B:41:HIS:CE1	1:B:42:VAL:HG23	2.52	0.44
1:A:287:ILE:HD13	1:A:287:ILE:HG21	1.50	0.44
1:A:352:GLY:O	1:A:377:VAL:N	2.37	0.44
1:B:237:GLN:HE21	1:B:237:GLN:HB2	1.42	0.44
1:B:303:ILE:CD1	1:B:334:ALA:HB3	2.48	0.44
1:B:35:ALA:HB2	1:B:54:ALA:HB2	1.99	0.44
1:B:315:ILE:HD11	1:B:321:LEU:CD1	2.47	0.44
1:B:1:MET:HE1	1:B:313:LEU:CB	2.45	0.44
1:A:82:TYR:CZ	1:A:295:VAL:HG22	2.52	0.44
1:B:55:PRO:HG2	1:B:58:LYS:HE3	1.99	0.44
1:A:170:ARG:HH11	1:A:181:SER:CB	2.29	0.44
1:A:346:THR:O	1:A:347:PHE:HB2	2.17	0.44
1:B:63:ILE:N	1:B:64:PRO:CD	2.81	0.44
1:B:63:ILE:N	1:B:64:PRO:HD2	2.33	0.43
1:A:36:ASP:OD2	1:A:60:TYR:OH	2.32	0.43
1:B:287:ILE:HG22	1:B:288:GLU:HG2	2.01	0.43
1:B:148:ILE:CG2	1:B:149:ALA:H	2.23	0.43
1:A:63:ILE:HG23	1:A:91:PHE:CD1	2.53	0.43
1:B:315:ILE:HD11	1:B:321:LEU:HD11	2.01	0.43
1:A:167:ARG:HG2	1:A:168:GLY:O	2.18	0.43
1:A:446:LEU:N	1:A:446:LEU:HD13	2.34	0.43
1:A:32:HIS:CE1	1:A:48:THR:HG23	2.53	0.43
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.95	0.43
1:B:280:GLU:O	1:B:281:ASN:HB2	2.19	0.42
1:B:149:ALA:HA	1:B:200:MET:HE1	2.01	0.42
1:B:62:ASN:ND2	1:B:65:ALA:HB2	2.35	0.42
1:B:48:THR:HG23	1:B:49:VAL:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:148:ILE:HG12	1:B:200:MET:HE1	2.02	0.42
1:A:24:LEU:HA	1:A:24:LEU:HD12	1.54	0.42
1:A:212:ILE:HD13	1:A:277:PHE:CE2	2.54	0.42
1:B:156:VAL:CG1	1:B:157:ILE:N	2.81	0.42
1:B:206:ASN:N	1:B:280:GLU:OE2	2.41	0.42
1:B:326:GLU:H	1:B:326:GLU:HG3	1.33	0.42
1:A:77:ALA:HB2	1:A:101:ILE:HB	2.02	0.42
1:A:208:ARG:NH2	1:A:246:PRO:O	2.35	0.42
1:A:244:PRO:HD2	1:A:333:HIS:ND1	2.35	0.42
1:A:274:THR:HG22	1:A:275:PHE:N	2.35	0.42
1:B:384:MET:CE	1:B:387:LYS:CG	2.98	0.42
1:A:32:HIS:HE1	1:A:48:THR:HG23	1.84	0.42
1:B:61:LEU:HD23	1:B:85:LEU:HD13	2.01	0.42
1:B:133:GLY:HA2	1:B:152:ILE:CD1	2.50	0.42
1:B:287:ILE:HD13	1:B:287:ILE:HG21	1.78	0.42
1:B:321:LEU:HA	1:B:321:LEU:HD12	1.73	0.42
1:A:152:ILE:HG13	1:A:202:LYS:HB2	2.01	0.42
1:B:123:MET:HG2	1:B:128:VAL:HB	1.99	0.42
1:B:61:LEU:CD2	1:B:85:LEU:HD13	2.50	0.42
1:A:333:HIS:CE1	1:A:395:ARG:HD2	2.55	0.42
1:A:9:ASN:OD1	1:A:10:ARG:N	2.50	0.42
1:A:22:LYS:NZ	1:B:407:GLN:OE1	2.51	0.42
1:A:353:LYS:HG3	1:A:376:THR:OG1	2.19	0.42
1:A:177:GLU:H	1:A:177:GLU:HG3	1.42	0.42
1:A:43:LEU:CD1	1:A:43:LEU:N	2.83	0.41
1:A:16:ARG:CG	1:A:309:ILE:HD12	2.50	0.41
1:B:260:CYS:SG	1:B:277:PHE:HZ	2.43	0.41
1:A:243:ALA:O	1:A:303:ILE:HD13	2.20	0.41
1:A:78:ILE:C	1:A:103:ILE:HD12	2.40	0.41
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.74	0.41
1:B:230:CYS:CB	1:B:238:LYS:HD3	2.50	0.41
1:B:243:ALA:HA	1:B:244:PRO:C	2.40	0.41
1:A:228:ARG:CD	1:A:299:VAL:CG1	2.98	0.41
1:A:16:ARG:HG3	1:A:309:ILE:HD12	2.02	0.41
1:B:1:MET:CE	1:B:2:LEU:HD12	2.50	0.41
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.90	0.41
1:A:328:VAL:O	1:A:329:HIS:CD2	2.73	0.41
1:A:313:LEU:HA	1:A:313:LEU:HD12	1.72	0.41
1:A:12:GLU:HB3	3:A:1000:HOH:O	2.20	0.41
1:B:157:ILE:O	1:B:157:ILE:HG23	2.21	0.41
1:B:202:LYS:CG	1:B:203:TYR:N	2.79	0.41
1:B:148:ILE:CG2	1:B:149:ALA:N	2.79	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:156:VAL:HG13	1:B:201:GLU:O	2.21	0.41
1:A:295:VAL:HG13	1:A:387:LYS:HE3	2.03	0.41
1:A:68:SER:OG	1:A:69:ALA:N	2.53	0.41
1:A:252:LEU:HD22	1:A:284:PHE:HE2	1.86	0.41
1:A:303:ILE:HD12	1:A:334:ALA:HB2	2.02	0.41
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.79	0.41
1:B:13:ILE:HB	1:B:82:TYR:CE2	2.56	0.41
1:B:223:ILE:HA	3:B:972:HOH:O	2.21	0.41
1:B:156:VAL:CG1	1:B:200:MET:CG	2.99	0.41
1:B:338:ARG:O	1:B:417:ASN:ND2	2.54	0.40
1:B:123:MET:HG3	1:B:128:VAL:CB	2.51	0.40
1:B:80:PRO:HB2	1:B:86:SER:HA	2.04	0.40
1:A:239:VAL:HG12	1:A:240:VAL:HG23	2.03	0.40
1:B:176:ALA:C	1:B:178:LEU:H	2.23	0.40
1:A:343:ASP:HB3	1:A:346:THR:OG1	2.21	0.40
1:A:292:ARG:NH1	1:A:294:GLN:HG2	2.36	0.40
1:B:403:LYS:NZ	1:B:431:GLN:HE22	2.19	0.40
1:B:129:PRO:HB2	1:B:284:PHE:O	2.21	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	427/449 (95%)	404 (95%)	23 (5%)	0	100	100
1	B	416/449 (93%)	387 (93%)	29 (7%)	0	100	100
All	All	843/898 (94%)	791 (94%)	52 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	352/361 (98%)	294 (84%)	58 (16%)	3	3
1	B	338/361 (94%)	283 (84%)	55 (16%)	3	4
All	All	690/722 (96%)	577 (84%)	113 (16%)	3	4

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ARG
1	A	24	LEU
1	A	39	LEU
1	A	40	LYS
1	A	43	LEU
1	A	44	LEU
1	A	57	VAL
1	A	68	SER
1	A	82	TYR
1	A	85	LEU
1	A	86	SER
1	A	97	ARG
1	A	98	SER
1	A	115	ASP
1	A	116	LYS
1	A	118	SER
1	A	120	ILE
1	A	123	MET
1	A	142	MET
1	A	146	ARG
1	A	152	ILE
1	A	167	ARG
1	A	169	MET
1	A	170	ARG
1	A	177	GLU
1	A	181	SER
1	A	200	MET
1	A	223	ILE

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Mol	Chain	Res	Type
1	A	227	GLU
1	A	232	MET
1	A	237	GLN
1	A	262	LYS
1	A	267	ILE
1	A	270	ARG
1	A	296	GLU
1	A	299	VAL
1	A	303	ILE
1	A	308	LEU
1	A	311	GLU
1	A	313	LEU
1	A	321	LEU
1	A	323	ILE
1	A	326	GLU
1	A	348	LEU
1	A	350	SER
1	A	387	LYS
1	A	393	GLU
1	A	394	ASN
1	A	403	LYS
1	A	407	GLN
1	A	415	LYS
1	A	416	THR
1	A	417	ASN
1	A	419	ASP
1	A	431	GLN
1	A	441	GLU
1	A	446	LEU
1	B	2	LEU
1	B	5	ILE
1	B	12	GLU
1	B	24	LEU
1	B	27	LYS
1	B	39	LEU
1	B	40	LYS
1	B	43	LEU
1	B	44	LEU
1	B	48	THR
1	B	56	SER
1	B	67	ILE
1	B	72	ILE

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Mol	Chain	Res	Type
1	B	76	VAL
1	B	84	PHE
1	B	85	LEU
1	B	86	SER
1	B	98	SER
1	B	116	LYS
1	B	123	MET
1	B	125	LYS
1	B	142	MET
1	B	143	ASP
1	B	146	ARG
1	B	148	ILE
1	B	175	ASP
1	B	178	LEU
1	B	181	SER
1	B	202	LYS
1	B	208	ARG
1	B	223	ILE
1	B	225	LEU
1	B	227	GLU
1	B	230	CYS
1	B	234	ARG
1	B	235	ARG
1	B	237	GLN
1	B	267	ILE
1	B	270	ARG
1	B	299	VAL
1	B	303	ILE
1	B	308	LEU
1	B	313	LEU
1	B	314	ARG
1	B	319	GLN
1	B	322	SER
1	B	326	GLU
1	B	342	GLU
1	B	348	LEU
1	B	382	ASP
1	B	410	ILE
1	B	415	LYS
1	B	444	LEU
1	B	446	LEU
1	B	447	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	180	GLN
1	A	206	ASN
1	A	290	ASN
1	A	340	ASN
1	A	404	ASN
1	A	417	ASN
1	B	32	HIS
1	B	145	ASN
1	B	237	GLN
1	B	290	ASN
1	B	333	HIS
1	B	345	ASN
1	B	404	ASN
1	B	417	ASN
1	B	429	ASN
1	B	431	GLN
1	B	447	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	953	-	4,4,4	1.87	1 (25%)	6,6,6	0.31	0
2	PO4	B	954	-	4,4,4	1.77	1 (25%)	6,6,6	0.31	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	953	-	-	0/0/0/0	0/0/0/0
2	PO4	B	954	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	953	PO4	P-O3	-2.84	1.41	1.52
2	B	954	PO4	P-O3	-2.41	1.43	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.