



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:02 PM UTC

PDB ID : 1BNC / pdb_00001bnc
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 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

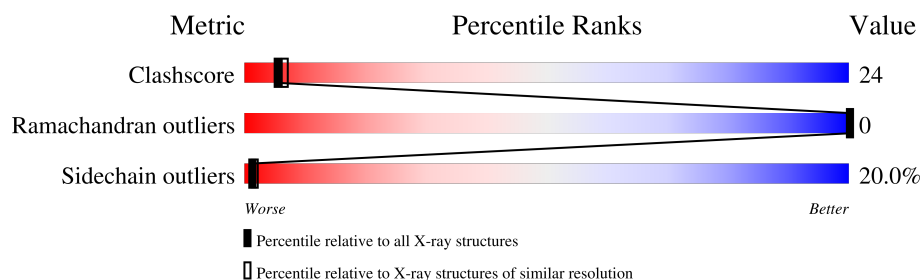
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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	B	954	-	X	X	-

2 Entry composition [i](#)

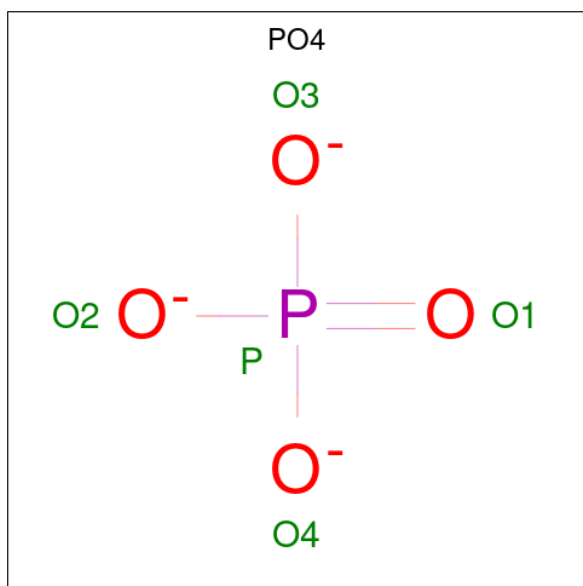
There are 3 unique types of molecules in this entry. The entry contains 6743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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			

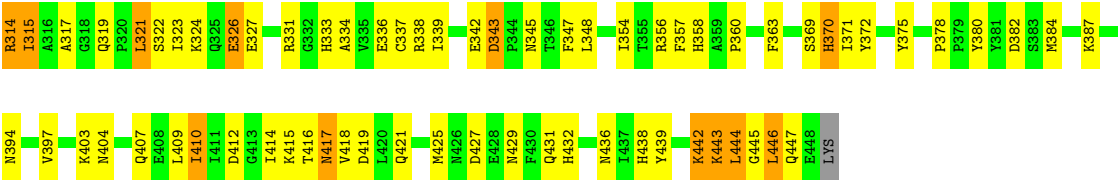
- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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	66	Total	O	0	0
			66	66		
3	B	50	Total	O	0	0
			50	50		



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	61.90Å 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 [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	3/3416 (0.1%)	1.69	49/4609 (1.1%)
1	B	1.23	8/3318 (0.2%)	1.65	36/4480 (0.8%)
All	All	1.24	11/6734 (0.2%)	1.67	85/9089 (0.9%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	ILE	CA-C	-6.36	1.46	1.53
1	A	378	PRO	C-N	-6.24	1.28	1.33
1	A	329	HIS	CE1-NE2	6.10	1.38	1.32
1	B	432	HIS	CE1-NE2	6.03	1.38	1.32
1	A	329	HIS	ND1-CE1	-5.82	1.26	1.32
1	B	363	PHE	N-CA	-5.55	1.39	1.46
1	B	90	ASN	CA-C	-5.39	1.46	1.52
1	B	287	ILE	CA-C	-5.37	1.47	1.52
1	B	297	HIS	CE1-NE2	5.24	1.37	1.32
1	B	314	ARG	C-N	-5.09	1.27	1.33
1	B	418	VAL	CA-CB	-5.08	1.49	1.54

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ILE	CB-CA-C	-13.72	98.84	111.05
1	A	287	ILE	CB-CA-C	-12.37	100.04	111.05
1	A	417	ASN	N-CA-CB	-11.41	93.81	110.80
1	A	267	ILE	N-CA-CB	-10.56	98.64	112.26
1	A	329	HIS	CA-CB-CG	-9.29	104.51	113.80
1	B	418	VAL	N-CA-C	7.96	118.50	110.23
1	B	417	ASN	N-CA-CB	-7.91	97.12	110.41
1	A	417	ASN	CA-CB-CG	7.86	120.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASP	CA-CB-CG	7.86	120.45	112.60
1	A	423	ARG	N-CA-CB	-7.70	98.36	110.22
1	B	208	ARG	N-CA-CB	7.64	122.62	110.85
1	A	198	VAL	N-CA-C	7.20	120.22	108.99
1	A	303	ILE	CA-CB-CG2	7.11	122.59	110.50
1	A	83	GLY	CA-C-N	-7.10	107.97	121.54
1	A	83	GLY	C-N-CA	-7.10	107.97	121.54
1	B	394	ASN	CB-CA-C	-7.09	96.27	110.30
1	B	79	HIS	CA-C-N	7.00	126.98	119.28
1	B	79	HIS	C-N-CA	7.00	126.98	119.28
1	A	223	ILE	CA-CB-CG2	6.85	122.15	110.50
1	B	380	TYR	N-CA-C	6.70	118.24	111.07
1	A	28	THR	N-CA-C	6.66	119.79	109.07
1	A	72	ILE	N-CA-C	6.65	117.40	110.62
1	A	168	GLY	N-CA-C	-6.55	102.64	111.54
1	B	287	ILE	O-C-N	6.44	126.94	121.98
1	A	67	ILE	N-CA-C	6.33	116.49	110.42
1	B	432	HIS	CA-CB-CG	-6.31	107.49	113.80
1	B	397	VAL	CA-C-N	6.24	128.64	120.28
1	B	397	VAL	C-N-CA	6.24	128.64	120.28
1	A	170	ARG	N-CA-C	6.16	119.16	108.76
1	A	427	ASP	CA-C-N	5.99	128.63	120.54
1	A	427	ASP	C-N-CA	5.99	128.63	120.54
1	B	417	ASN	CB-CA-C	-5.95	98.11	109.95
1	A	377	VAL	CA-C-N	5.92	126.48	120.38
1	A	377	VAL	C-N-CA	5.92	126.48	120.38
1	B	303	ILE	CA-CB-CG2	5.91	120.56	110.50
1	A	175	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	418	VAL	N-CA-C	5.87	116.53	110.36
1	B	358	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	378	PRO	CB-CA-C	-5.81	103.83	110.92
1	B	233	GLN	N-CA-C	5.75	118.44	109.52
1	A	384	MET	N-CA-C	5.72	118.01	109.25
1	A	267	ILE	CB-CG1-CD1	-5.69	101.84	113.80
1	B	419	ASP	CA-CB-CG	-5.61	106.99	112.60
1	B	123	MET	CA-CB-CG	-5.57	102.97	114.10
1	A	90	ASN	O-C-N	5.55	128.03	122.03
1	B	416	THR	CA-C-N	5.53	132.35	121.58
1	B	416	THR	C-N-CA	5.53	132.35	121.58
1	B	343	ASP	CA-C-O	5.50	123.70	119.46
1	B	378	PRO	CA-C-N	5.49	125.19	119.64
1	B	378	PRO	C-N-CA	5.49	125.19	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	HIS	CA-CB-CG	-5.48	108.32	113.80
1	B	345	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	63	ILE	CA-C-O	5.44	122.84	118.71
1	B	354	ILE	CB-CA-C	-5.43	104.73	111.08
1	A	3	ASP	N-CA-C	5.42	117.05	111.03
1	B	85	LEU	CA-C-N	5.42	127.81	120.38
1	B	85	LEU	C-N-CA	5.42	127.81	120.38
1	A	299	VAL	CB-CA-C	5.38	119.40	112.14
1	A	28	THR	CA-C-N	-5.37	116.54	123.19
1	A	28	THR	C-N-CA	-5.37	116.54	123.19
1	A	431	GLN	N-CA-CB	5.33	118.53	110.28
1	B	213	GLN	CA-C-N	-5.28	115.32	122.92
1	B	213	GLN	C-N-CA	-5.28	115.32	122.92
1	A	425	MET	N-CA-C	-5.24	105.74	111.82
1	A	108	GLU	CB-CA-C	-5.23	102.44	110.81
1	A	227	GLU	CB-CG-CD	5.23	121.49	112.60
1	B	101	ILE	CB-CA-C	-5.22	103.34	110.96
1	A	379	PRO	CB-CA-C	-5.22	103.52	110.88
1	A	309	ILE	CA-CB-CG1	-5.21	101.55	110.40
1	B	172	VAL	N-CA-C	5.14	115.37	108.17
1	A	303	ILE	CB-CA-C	5.12	120.51	112.16
1	A	320	PRO	N-CA-CB	5.12	108.63	103.25
1	A	394	ASN	N-CA-CB	5.10	119.82	111.31
1	B	205	GLU	N-CA-C	5.10	116.52	111.07
1	A	57	VAL	CB-CA-C	-5.09	104.27	112.16
1	A	267	ILE	CA-CB-CG1	5.08	119.04	110.40
1	A	72	ILE	CB-CA-C	-5.08	105.29	112.14
1	A	306	VAL	CB-CA-C	-5.08	104.25	111.21
1	A	309	ILE	N-CA-C	5.04	116.49	111.00
1	A	303	ILE	N-CA-C	5.03	118.19	111.44
1	B	3	ASP	N-CA-CB	-5.03	102.68	110.07
1	A	362	GLY	CA-C-N	5.02	128.45	121.02
1	A	362	GLY	C-N-CA	5.02	128.45	121.02
1	B	99	GLY	CA-C-N	-5.02	113.76	122.64
1	B	99	GLY	C-N-CA	-5.02	113.76	122.64

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	3356	0	3391	148	0
1	B	3261	0	3260	169	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	316	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 24.

All (316) 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: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:1:MET:HE2	1:B:313:LEU:HB3	1.56	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:A:275:PHE:CE1	1:A:289:MET:HE3	2.16	0.80
1:B:1:MET:HE3	1:B:26:ILE:HD11	1.65	0.79
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:A:427:ASP:O	1:A:431:GLN:HG3	1.85	0.77
1:B:263:ALA:O	1:B:267:ILE:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:HD11	1:B:334:ALA:N	1.99	0.76
1:A:112:LEU:CD1	1:A:118:SER:HB2	2.18	0.74
1:B:149:ALA:CA	1:B:200:MET:HE1	2.17	0.74
1:B:113:MET:HE2	1:B:267:ILE:HD12	1.69	0.72
1:A:1:MET:HE2	1:A:317:ALA:HB2	1.72	0.72
1:A:275:PHE:CZ	1:A:289:MET:HE3	2.24	0.72
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:B:1:MET:HE3	1:B:26:ILE:CD1	2.21	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
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:159:LYS:N	1:A:199:TYR:O	2.27	0.66
1:A:339:ILE:HA	1:A:417:ASN:ND2	2.10	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:113:MET:HE3	1:B:267:ILE:HD12	1.79	0.65
1:B:149:ALA:HA	1:B:200:MET:HE1	1.78	0.65
1:A:170:ARG:NH1	1:A:181:SER:OG	2.29	0.65
1:B:1:MET:SD	1:B:317:ALA:HB2	2.36	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:A:112:LEU:HG	1:A:113:MET:HE2	1.79	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:149:ALA:N	1:B:200:MET:HE1	2.17	0.60
1:B:303:ILE:HD11	1:B:333:HIS:C	2.26	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: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:56:SER:HG	1:A:84:PHE:HE1	1.48	0.59
1:A:123:MET:HE3	1:A:128:VAL:CG2	2.33	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
1:B:384:MET:HE2	1:B:387:LYS:HG3	1.86	0.58
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:A:217:ASP:OD2	1:A:221:ASN:ND2	2.23	0.57
1:B:286:PHE:CZ	1:B:288:GLU:HA	2.39	0.57
1:B:104:GLY:O	1:B:270:ARG:NH1	2.37	0.57
1:A:93:GLU:CD	1:A:111:ARG:HH22	2.13	0.57
1:B:175:ASP:OD1	1:B:175:ASP:N	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:OE1	1:B:421:GLN:HA	2.06	0.56
1:A:339:ILE:HA	1:A:417:ASN:HD21	1.70	0.56
1:A:32:HIS:O	1:A:50:CYS:HA	2.06	0.56
1:B:241:GLU:HG2	1:B:296:GLU:HG2	1.88	0.56
1:B:245:ALA:HB3	1:B:248:ILE:HG13	1.86	0.56
1:B:120:ILE:CG2	1:B:124:LYS:HD2	2.35	0.56
1:A:128:VAL:HG13	1:A:129:PRO:HD2	1.89	0.55
1:A:63:ILE:HB	1:A:64:PRO:HD3	1.88	0.55
1:B:148:ILE:O	1:B:151:ARG:HB3	2.06	0.55
1:A:376:THR:O	1:A:378:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:OE1	1:B:336:GLU:OE2	2.25	0.55
1:A:303:ILE:HD11	1:A:333:HIS:C	2.32	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:2:LEU:O	1:B:26:ILE:HG12	2.07	0.54
1:B:410:ILE:O	1:B:410:ILE:HG22	2.05	0.54
1:B:68:SER:O	1:B:71:GLU:HB2	2.08	0.54
1:A:4:LYS:NZ	1:A:47:GLU:OE2	2.41	0.54
1:A:39:LEU:HD23	1:A:41:HIS:HE1	1.73	0.54
1:B:149:ALA:HA	1:B:200:MET:CE	2.37	0.54
1:B:303:ILE:HD12	1:B:334:ALA:CB	2.38	0.54
1:B:442:LYS:O	1:B:445:GLY:N	2.40	0.54
1:B:177:GLU:O	1:B:181:SER:HB2	2.08	0.53
1:B:331:ARG:NH2	3:B:1002:HOH:O	2.40	0.53
1:A:113:MET:HE1	1:A:122:ALA:HB3	1.89	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:A:232:MET:HE2	1:A:430:PHE:CD1	2.43	0.53
1:A:241:GLU:OE1	1:A:336:GLU:OE2	2.27	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:B:337:CYS:SG	1:B:425:MET:HE3	2.48	0.53
1:A:297:HIS:CG	1:A:298:PRO:HD3	2.44	0.52
1:A:350:SER:O	1:A:350:SER:OG	2.28	0.52
1:B:384:MET:HE2	1:B:387:LYS:CG	2.40	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:211:GLU:HG3	1:A:274:THR:HG21	1.91	0.52
1:B:370:HIS:ND1	1:B:370:HIS:N	2.46	0.52
1:A:441:GLU:HG2	1:A:446:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:HB3	1:A:39:LEU:HD22	1.91	0.51
1:B:134:SER:HA	1:B:148:ILE:CD1	2.39	0.51
1:A:138:LEU:HD21	1:A:200:MET:CE	2.41	0.51
1:B:384:MET:HE1	1:B:387:LYS:HG2	1.93	0.51
1:B:53:PRO:C	1:B:55:PRO:HD2	2.35	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: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:384:MET:CE	1:B:387:LYS:HG2	2.41	0.50
1:B:63:ILE:CB	1:B:64:PRO:HD3	2.42	0.50
1:B:16:ARG:HD3	3:B:981:HOH:O	2.12	0.50
1:A:245:ALA:HB3	1:A:248:ILE:HG13	1.92	0.49
1:B:16:ARG:NE	1:B:309:ILE:HD13	2.26	0.49
1:A:241:GLU:CD	1:A:296:GLU:HG2	2.37	0.49
1:A:214:VAL:HG22	1:A:273:GLY:O	2.13	0.49
1:A:228:ARG:HD3	1:A:299:VAL:HG12	1.93	0.49
1:A:187:ALA:O	1:A:190:LYS:O	2.30	0.49
1:A:223:ILE:HG12	1:A:325:GLN:OE1	2.12	0.49
1:B:427:ASP:OD2	1:B:439:TYR:OH	2.29	0.49
1:A:63:ILE:N	1:A:64:PRO:CD	2.76	0.48
1:A:148:ILE:O	1:A:151:ARG:HB3	2.13	0.48
1:B:144:LYS:O	1:B:147:ALA:N	2.45	0.48
1:B:43:LEU:CD1	1:B:43:LEU:N	2.77	0.48
1:B:303:ILE:HD12	1:B:334:ALA:HB3	1.95	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:A:338:ARG:HD3	1:A:384:MET:CE	2.44	0.48
1:B:4:LYS:NZ	1:B:47:GLU:OE1	2.43	0.48
1:B:32:HIS:HD2	1:B:33:SER:O	1.96	0.48
1:B:113:MET:HE1	1:B:123:MET:HE1	1.94	0.48
1:B:175:ASP:HA	1:B:178:LEU:HD22	1.95	0.48
1:A:249:THR:HB	1:A:250:PRO:HD2	1.95	0.48
1:B:78:ILE:O	1:B:80:PRO:HD3	2.14	0.48
1:B:131:VAL:HG22	1:B:285:TYR:HB3	1.95	0.48
1:B:1:MET:HE1	1:B:2:LEU:HD12	1.96	0.48
1:A:215:LEU:O	1:A:222:ALA:HA	2.13	0.47
1:B:372:TYR:O	1:B:375:TYR:HB3	2.14	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:A:138:LEU:HD21	1:A:200:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:211:GLU:HG3	1:A:274:THR:CG2	2.45	0.47
1:B:89:ALA:O	1:B:93:GLU:HB2	2.14	0.47
1:B:427:ASP:OD1	1:B:429:ASN:N	2.47	0.47
1:B:15:LEU:O	1:B:19:ARG:HG3	2.15	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:A:78:ILE:C	1:A:103:ILE:HD12	2.40	0.46
1:A:372:TYR:O	1:A:375:TYR:HB3	2.15	0.46
1:B:56:SER:HA	1:B:59:SER:OG	2.16	0.46
1:A:297:HIS:N	1:A:298:PRO:CD	2.79	0.46
1:B:339:ILE:HA	1:B:417:ASN:HD22	1.80	0.46
1:A:267:ILE:HG21	1:A:267:ILE:HD13	1.29	0.46
1:B:243:ALA:HA	1:B:244:PRO:C	2.40	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
1:A:123:MET:HE3	1:A:128:VAL:HB	1.99	0.45
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:176:ALA:C	1:B:178:LEU:H	2.23	0.45
1:A:39:LEU:HD12	1:A:39:LEU:HA	1.60	0.45
1:B:101:ILE:O	1:B:101:ILE:HG22	2.12	0.45
1:B:241:GLU:OE2	1:B:338:ARG:NE	2.36	0.45
1:A:82:TYR:CD1	1:A:82:TYR:C	2.95	0.45
1:A:306:VAL:HG12	1:A:307:ASP:N	2.32	0.45
1:A:370:HIS:ND1	1:A:370:HIS:N	2.61	0.45
1:B:54:ALA:N	1:B:55:PRO:CD	2.79	0.45
1:B:303:ILE:CD1	1:B:334:ALA:CB	2.95	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:85:LEU:HB3	1:A:91:PHE:CD2	2.52	0.44
1:A:287:ILE:HG21	1:A:287:ILE:HD13	1.50	0.44
1:A:352:GLY:O	1:A:377:VAL:N	2.37	0.44
1:B:41:HIS:CE1	1:B:42:VAL:HG23	2.52	0.44
1:B:237:GLN:HE21	1:B:237:GLN:HB2	1.42	0.44
1:B:35:ALA:HB2	1:B:54:ALA:HB2	1.99	0.44
1:B:303:ILE:CD1	1:B:334:ALA:HB3	2.48	0.44
1:B:315:ILE:HD11	1:B:321:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:CZ	1:A:295:VAL:HG22	2.52	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:55:PRO:HG2	1:B:58:LYS:HE3	1.99	0.44
1:A:120:ILE:HG22	1:A:121:ALA:N	2.26	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:B:97:ARG:C	1:B:99:GLY:H	2.26	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:A:63:ILE:HG23	1:A:91:PHE:CD1	2.53	0.43
1:A:167:ARG:HG2	1:A:168:GLY:O	2.18	0.43
1:B:148:ILE:CG2	1:B:149:ALA:H	2.23	0.43
1:B:315:ILE:HD11	1:B:321:LEU:HD11	2.01	0.43
1:A:123:MET:HE3	1:A:128:VAL:HG21	1.90	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:B:77:ALA:C	1:B:78:ILE:HG12	2.44	0.43
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.95	0.43
1:B:48:THR:C	1:B:49:VAL:HG23	2.43	0.42
1:B:280:GLU:O	1:B:281:ASN:HB2	2.19	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
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.54	0.42
1:A:212:ILE:HD13	1:A:277:PHE:CE2	2.54	0.42
1:A:232:MET:HE3	1:A:424:ILE:HG23	2.01	0.42
1:B:209:HIS:ND1	1:B:209:HIS:C	2.77	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: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:32:HIS:HE1	1:A:48:THR:HG23	1.84	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: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:A:152:ILE:HG13	1:A:202:LYS:HB2	2.01	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:B:61:LEU:CD2	1:B:85:LEU:HD13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HG2	1:B:128:VAL:HB	1.99	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:333:HIS:CE1	1:A:395:ARG:HD2	2.55	0.42
1:A:177:GLU:H	1:A:177:GLU:HG3	1.42	0.42
1:A:353:LYS:HG3	1:A:376:THR:OG1	2.19	0.42
1:A:16:ARG:CG	1:A:309:ILE:HD12	2.50	0.41
1:A:43:LEU:N	1:A:43:LEU:CD1	2.83	0.41
1:B:1:MET:HE1	1:B:2:LEU:CD1	2.49	0.41
1:B:260:CYS:SG	1:B:277:PHE:HZ	2.43	0.41
1:B:436:ASN:C	1:B:438:HIS:N	2.78	0.41
1:A:243:ALA:O	1:A:303:ILE:HD13	2.20	0.41
1:B:230:CYS:CB	1:B:238:LYS:HD3	2.50	0.41
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.74	0.41
1:A:16:ARG:HG3	1:A:309:ILE:HD12	2.02	0.41
1:A:228:ARG:CD	1:A:299:VAL:CG1	2.98	0.41
1:A:339:ILE:C	1:A:340:ASN:HD22	2.28	0.41
1:A:328:VAL:O	1:A:329:HIS:CD2	2.73	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:12:GLU:HB3	3:A:1000:HOH:O	2.20	0.41
1:A:209:HIS:CD2	1:A:209:HIS:C	2.98	0.41
1:A:275:PHE:CE1	1:A:289:MET:CE	2.99	0.41
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.72	0.41
1:B:276:GLU:CD	1:B:290:ASN:HD21	2.29	0.41
1:B:384:MET:CE	1:B:387:LYS:CG	2.98	0.41
1:B:157:ILE:C	1:B:158:ILE:HD13	2.45	0.41
1:B:157:ILE:O	1:B:157:ILE:HG23	2.21	0.41
1:B:296:GLU:C	1:B:298:PRO:HD2	2.46	0.41
1:A:68:SER:OG	1:A:69:ALA:N	2.53	0.41
1:A:295:VAL:HG13	1:A:387:LYS:HE3	2.03	0.41
1:B:156:VAL:HG13	1:B:201:GLU:O	2.21	0.41
1:B:202:LYS:CG	1:B:203:TYR:N	2.79	0.41
1:A:1:MET:HE2	1:A:317:ALA:CB	2.48	0.41
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.79	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: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:A:239:VAL:HG12	1:A:240:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PRO:HB2	1:B:86:SER:HA	2.04	0.40
1:B:123:MET:HG3	1:B:128:VAL:CB	2.51	0.40
1:B:338:ARG:O	1:B:417:ASN:ND2	2.54	0.40
1:A:123:MET:HE3	1:A:128:VAL:CB	2.51	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:129:PRO:HB2	1:B:284:PHE:O	2.21	0.40
1:B:403:LYS:NZ	1:B:431:GLN:HE22	2.19	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	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 [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%)	281 (80%)	71 (20%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	338/361 (94%)	271 (80%)	67 (20%)	1	2
All	All	690/722 (96%)	552 (80%)	138 (20%)	1	2

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ARG
1	A	22	LYS
1	A	24	LEU
1	A	39	LEU
1	A	43	LEU
1	A	44	LEU
1	A	48	THR
1	A	57	VAL
1	A	67	ILE
1	A	68	SER
1	A	72	ILE
1	A	85	LEU
1	A	86	SER
1	A	97	ARG
1	A	98	SER
1	A	108	GLU
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	144	LYS
1	A	146	ARG
1	A	152	ILE
1	A	158	ILE
1	A	167	ARG
1	A	169	MET
1	A	170	ARG
1	A	171	VAL
1	A	177	GLU
1	A	181	SER
1	A	200	MET
1	A	223	ILE
1	A	227	GLU

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Mol	Chain	Res	Type
1	A	232	MET
1	A	237	GLN
1	A	256	ILE
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	324	LYS
1	A	326	GLU
1	A	339	ILE
1	A	348	LEU
1	A	350	SER
1	A	353	LYS
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	420	LEU
1	A	424	ILE
1	A	431	GLN
1	A	441	GLU
1	A	442	LYS
1	A	446	LEU
1	B	2	LEU
1	B	5	ILE
1	B	24	LEU
1	B	27	LYS
1	B	39	LEU
1	B	40	LYS
1	B	43	LEU

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Mol	Chain	Res	Type
1	B	44	LEU
1	B	48	THR
1	B	56	SER
1	B	58	LYS
1	B	67	ILE
1	B	72	ILE
1	B	76	VAL
1	B	78	ILE
1	B	85	LEU
1	B	86	SER
1	B	96	GLU
1	B	98	SER
1	B	101	ILE
1	B	116	LYS
1	B	123	MET
1	B	142	MET
1	B	143	ASP
1	B	146	ARG
1	B	148	ILE
1	B	150	LYS
1	B	152	ILE
1	B	158	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	262	LYS
1	B	267	ILE
1	B	270	ARG
1	B	299	VAL
1	B	303	ILE
1	B	308	LEU
1	B	309	ILE
1	B	313	LEU

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Mol	Chain	Res	Type
1	B	314	ARG
1	B	315	ILE
1	B	319	GLN
1	B	321	LEU
1	B	322	SER
1	B	323	ILE
1	B	326	GLU
1	B	342	GLU
1	B	348	LEU
1	B	382	ASP
1	B	410	ILE
1	B	414	ILE
1	B	415	LYS
1	B	442	LYS
1	B	443	LYS
1	B	444	LEU
1	B	446	LEU
1	B	447	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	180	GLN
1	A	206	ASN
1	A	209	HIS
1	A	233	GLN
1	A	404	ASN
1	A	417	ASN
1	A	432	HIS
1	B	32	HIS
1	B	145	ASN
1	B	219	GLN
1	B	237	GLN
1	B	290	ASN
1	B	333	HIS
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 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	953	-	4,4,4	3.11	3 (75%)	6,6,6	0.51	0
2	PO4	B	954	-	4,4,4	3.04	4 (100%)	6,6,6	0.53	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	953	PO4	P-O3	-4.59	1.41	1.54
2	B	954	PO4	P-O3	-3.98	1.43	1.54
2	A	953	PO4	P-O4	-3.18	1.45	1.54
2	B	954	PO4	P-O2	-2.98	1.46	1.54
2	B	954	PO4	P-O4	-2.65	1.46	1.54
2	A	953	PO4	P-O2	-2.38	1.47	1.54
2	B	954	PO4	P-O1	-2.27	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	953	PO4	1	0
2	B	954	PO4	2	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.