



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:27 PM EDT

PDB ID : 3N5F / pdb_00003n5f
Title : Crystal Structure of L-N-carbamoylase from *Geobacillus stearothermophilus* CECT43
Authors : Garcia-Pino, A.; Martinez-Rodriguez, S.; Gavira, J.A.
Deposited on : 2010-05-25
Resolution : 2.75 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

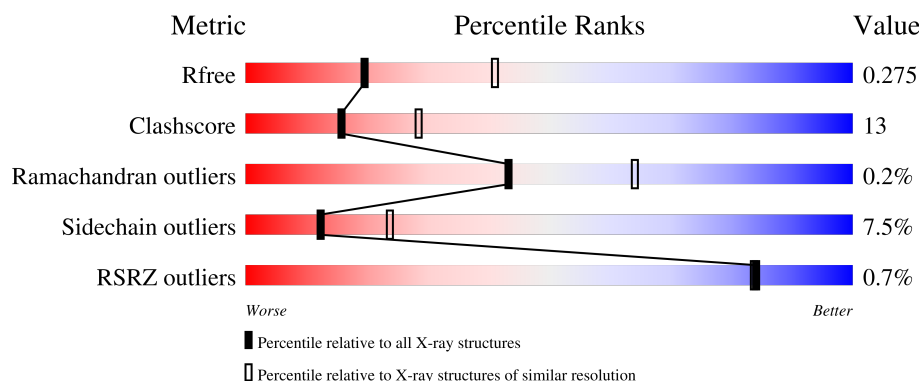
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	408	70% 26% •
1	B	408	75% 22% •

2 Entry composition [i](#)

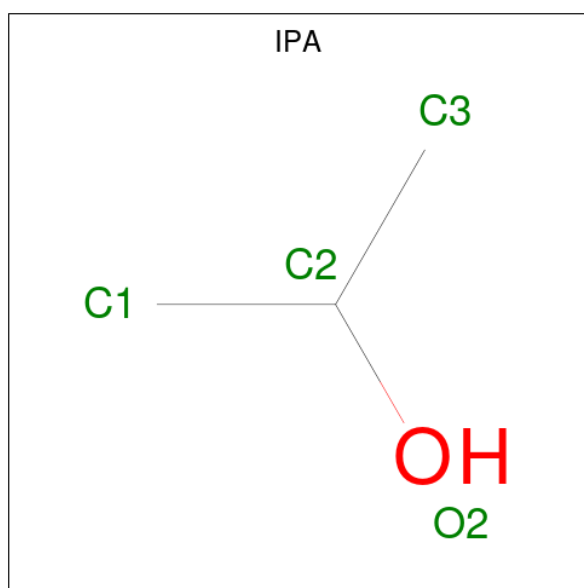
There are 5 unique types of molecules in this entry. The entry contains 6204 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-carbamoyl-L-amino acid hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	4	0
			3010	1905	526	562	17			
1	B	406	Total	C	N	O	S	0	6	0
			3051	1936	535	564	16			

- Molecule 2 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).

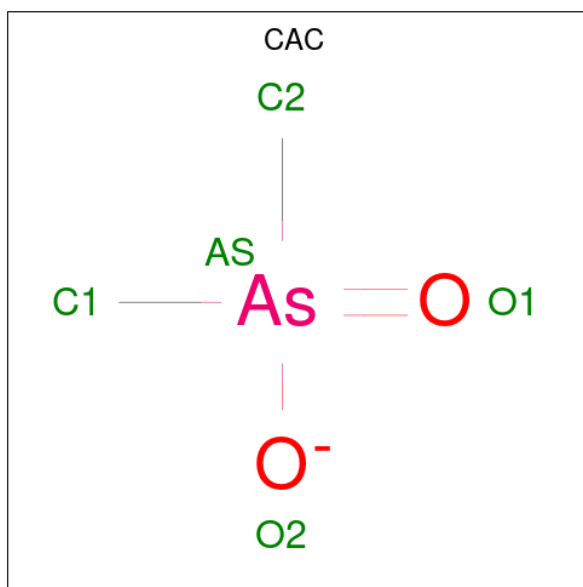


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		
2	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co 1 1	0	0
3	B	1	Total Co 1 1	0	0

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total As C O 5 1 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	47	Total O 47 47	0	0
5	B	81	Total O 81 81	0	0

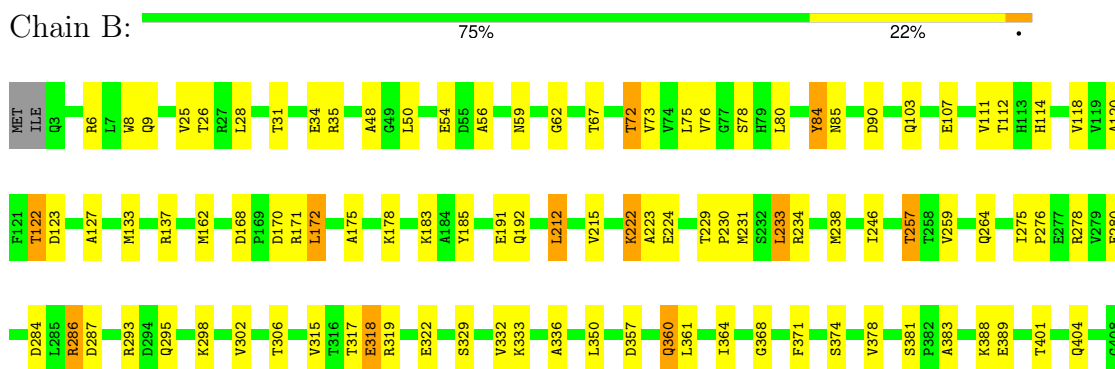
3 Residue-property plots [i](#)

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 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.

- Molecule 1: N-carbamoyl-L-amino acid hydrolase



- Molecule 1: N-carbamoyl-L-amino acid hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.21Å 211.68Å 43.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.75) 98.2 (20.00-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.193 , 0.276 0.194 , 0.275	Depositor DCC
R_{free} test set	1271 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6204	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, CAC, IPA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	0/3081	1.09	10/4193 (0.2%)
1	B	0.87	0/3127	1.05	6/4252 (0.1%)
All	All	0.84	0/6208	1.07	16/8445 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	CYS	N-CA-C	8.78	115.89	108.07
1	B	123	ASP	N-CA-C	6.87	119.60	111.02
1	B	84	TYR	N-CA-C	6.61	118.18	110.97
1	A	123	ASP	N-CA-C	6.19	118.75	111.02
1	A	72	THR	CB-CA-C	6.12	119.87	109.53
1	A	151	ARG	N-CA-C	5.86	119.02	109.59
1	B	84	TYR	CA-C-N	-5.76	113.92	123.37
1	B	84	TYR	C-N-CA	-5.76	113.92	123.37
1	A	17	VAL	N-CA-C	5.71	116.48	110.72
1	A	110	VAL	N-CA-C	5.38	115.85	107.99
1	B	73	VAL	N-CA-C	5.34	116.99	108.87
1	A	84	TYR	CA-C-N	-5.30	115.08	123.24
1	A	84	TYR	C-N-CA	-5.30	115.08	123.24
1	A	82	SER	N-CA-C	5.18	116.17	108.86
1	A	77	GLY	N-CA-C	5.17	119.91	111.27
1	B	6	ARG	NE-CZ-NH2	5.03	123.72	119.20

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	3010	0	2943	93	1
1	B	3051	0	3025	70	1
2	A	4	0	8	0	0
2	B	4	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	5	0	0	0	0
5	A	47	0	0	5	0
5	B	81	0	0	5	0
All	All	6204	0	5984	160	1

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 13.

All (160) 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:257:THR:HG22	1:B:287:ASP:OD2	1.41	1.19
1:A:64:LYS:NZ	1:A:105:MET:HB3	1.64	1.11
1:A:72:THR:HG23	1:A:183:LYS:HB2	1.32	1.07
1:A:72:THR:CG2	1:A:183:LYS:HB2	1.93	0.98
1:A:64:LYS:HZ2	1:A:105:MET:HB3	1.25	0.97
1:B:332:VAL:HG11	1:B:368:GLY:HA3	1.45	0.96
1:B:222:LYS:HD2	1:B:224:GLU:OE2	1.81	0.80
1:A:64:LYS:NZ	1:A:105:MET:CB	2.43	0.80
1:B:112:THR:HG23	1:B:114:HIS:O	1.81	0.79
1:A:265:LEU:HD22	1:A:281:PHE:HB3	1.64	0.79
1:B:9:GLN:NE2	5:B:431:HOH:O	2.15	0.78
1:A:42:ALA:HA	1:A:45:MET:HE2	1.67	0.77
1:A:6:ARG:O	1:A:10:ARG:HG3	1.86	0.76
1:A:168:ASP:OD2	1:A:170:ASP:OD2	2.05	0.75
1:B:133:MET:HE3	1:B:357:ASP:HA	1.68	0.75
1:B:67:THR:CG2	1:B:111[A]:VAL:CG1	2.66	0.74
1:B:332:VAL:CG1	1:B:368:GLY:HA3	2.17	0.73
1:A:130:ARG:HH21	1:A:151:ARG:H	1.34	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLU:OE1	1:B:229:THR:HG21	1.92	0.69
1:B:318[B]:GLU:OE2	5:B:489:HOH:O	2.12	0.68
1:B:259:VAL:CG2	1:B:286:ARG:HG3	2.24	0.67
1:A:162:MET:HE1	1:A:172:LEU:HD13	1.78	0.66
1:A:72:THR:HG23	1:A:183:LYS:CB	2.19	0.65
1:B:122:THR:OG1	5:B:483:HOH:O	1.69	0.64
1:B:67:THR:CG2	1:B:111[A]:VAL:HG12	2.28	0.64
1:A:154:GLU:OE2	1:A:154:GLU:CA	2.46	0.64
1:A:72:THR:HG22	1:A:114:HIS:CE1	2.33	0.64
1:A:3:GLN:NE2	5:A:418:HOH:O	2.30	0.63
1:B:35:ARG:NH2	1:B:54:GLU:OE2	2.32	0.62
1:A:64:LYS:HE3	1:A:106:ASN:OD1	2.00	0.62
1:B:257:THR:CG2	1:B:287:ASP:OD2	2.33	0.61
1:B:378:VAL:HG11	1:B:383:ALA:HB3	1.83	0.61
1:A:378:VAL:HG11	5:A:437:HOH:O	1.99	0.61
1:B:75:LEU:HB3	1:B:185:TYR:HD1	1.66	0.61
1:A:40:LEU:O	1:A:43:SER:HB3	2.01	0.61
1:B:332:VAL:HG11	1:B:368:GLY:CA	2.27	0.60
1:A:64:LYS:HZ2	1:A:105:MET:CB	2.03	0.60
1:A:75:LEU:HB3	1:A:185:TYR:HD1	1.66	0.60
1:B:72:THR:HG23	1:B:183:LYS:N	2.17	0.60
1:A:130:ARG:NH2	1:A:151:ARG:H	2.00	0.60
1:A:203:VAL:HG12	1:A:204:GLY:N	2.17	0.59
1:B:67:THR:HG22	1:B:111[A]:VAL:CG1	2.31	0.59
1:A:147:ALA:O	1:A:158:LEU:HD23	2.03	0.59
1:B:133:MET:O	1:B:137:ARG:HG3	2.03	0.58
1:A:85:ASN:O	1:A:381:SER:HA	2.03	0.58
1:B:56:ALA:HB3	1:B:175:ALA:HB2	1.85	0.57
1:A:41:VAL:HG23	1:A:60:LEU:CD2	2.35	0.56
1:B:212:LEU:N	1:B:293:ARG:HH11	2.02	0.56
1:A:35:ARG:HH22	1:A:54:GLU:CD	2.12	0.56
1:A:35:ARG:NH2	1:A:54:GLU:OE2	2.32	0.56
1:B:72:THR:CG2	1:B:183:LYS:HB2	2.36	0.56
1:B:259:VAL:HG23	1:B:286:ARG:HG3	1.86	0.55
1:A:154:GLU:OE2	1:A:154:GLU:HA	2.07	0.54
1:A:85:ASN:O	1:A:382:PRO:HD3	2.08	0.54
1:A:332:VAL:HG11	1:A:368:GLY:HA3	1.88	0.54
1:B:114:HIS:CE1	1:B:183:LYS:HD3	2.43	0.54
1:A:293:ARG:HG3	1:A:294:ASP:N	2.22	0.54
1:A:92:PRO:O	1:A:93:LEU:C	2.51	0.53
1:B:360:GLN:HG3	5:B:456:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:THR:OG1	1:B:84:TYR:O	2.26	0.52
1:B:9:GLN:OE1	5:B:485:HOH:O	2.19	0.51
1:A:114:HIS:CE1	1:A:183:LYS:HD2	2.46	0.51
1:B:48:ALA:CB	1:B:103:GLN:HB2	2.41	0.51
1:A:274:VAL:HG12	1:A:275:ILE:O	2.11	0.51
1:A:45:MET:HE3	1:A:52:VAL:HG22	1.93	0.51
1:A:293:ARG:NH1	1:A:294:ASP:OD1	2.43	0.51
1:A:331:GLU:HB2	5:A:455:HOH:O	2.10	0.51
1:A:393:ALA:O	1:A:397:VAL:HG23	2.11	0.51
1:A:378:VAL:CG1	5:A:437:HOH:O	2.56	0.50
1:A:398:LEU:O	1:A:402:VAL:HG23	2.12	0.50
1:A:213:ILE:HD11	1:A:285:LEU:HD23	1.93	0.50
1:B:85:ASN:O	1:B:381:SER:HA	2.11	0.50
1:B:298:LYS:O	1:B:302:VAL:HG23	2.11	0.50
1:A:75:LEU:HD22	1:A:119:VAL:CG1	2.42	0.49
1:B:224:GLU:OE1	1:B:229:THR:CG2	2.58	0.49
1:B:112:THR:CG2	1:B:114:HIS:O	2.56	0.49
1:B:231:MET:HA	1:B:234:ARG:HD2	1.95	0.49
1:A:38:LYS:O	1:A:39:ASP:C	2.55	0.49
1:B:329:SER:O	1:B:333:LYS:HG3	2.13	0.49
1:A:54:GLU:HG2	1:A:60:LEU:HD12	1.95	0.48
1:B:90:ASP:OD2	1:B:90:ASP:C	2.56	0.48
1:A:265:LEU:CD2	1:A:281:PHE:HB3	2.41	0.48
1:A:203:VAL:CG1	1:A:204:GLY:N	2.76	0.48
1:A:381:SER:O	1:A:384:GLU:HB2	2.13	0.48
1:A:328:CYS:O	1:A:333:LYS:HE2	2.13	0.47
1:A:373:ARG:HD2	1:A:390:ASP:OD2	2.14	0.47
1:A:157:SER:O	1:A:160:GLU:N	2.47	0.47
1:B:230:PRO:O	1:B:234:ARG:HG3	2.14	0.47
1:A:64:LYS:HZ3	1:A:105:MET:CB	2.27	0.47
1:A:76:VAL:O	1:A:118:VAL:HA	2.14	0.47
1:A:259:VAL:HG12	1:B:231:MET:HG2	1.97	0.47
1:A:45:MET:CE	1:A:52:VAL:HG13	2.45	0.46
1:B:284:ASP:OD1	1:B:284:ASP:C	2.58	0.46
1:A:41:VAL:HA	1:A:44:TYR:CD1	2.49	0.46
1:A:287:ASP:HB3	1:A:293:ARG:HB3	1.97	0.46
1:A:154:GLU:OE2	1:A:154:GLU:N	2.48	0.46
1:A:270:GLY:O	1:B:264[A]:GLN:HB2	2.14	0.46
1:B:191:GLU:O	1:B:192:GLN:HB2	2.16	0.46
1:B:264[A]:GLN:OE1	1:B:264[A]:GLN:HA	2.13	0.46
1:B:168:ASP:HB3	1:B:171:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG21	1:B:286:ARG:HG3	1.98	0.46
1:A:20:GLN:C	1:A:22:SER:N	2.74	0.45
1:B:48:ALA:HB2	1:B:103:GLN:HB2	1.99	0.45
1:B:54:GLU:HA	1:B:59:ASN:O	2.17	0.45
1:A:212:LEU:C	1:A:212:LEU:HD23	2.41	0.45
1:A:257:THR:OG1	1:A:287:ASP:OD2	2.33	0.45
1:A:77:GLY:HA3	1:A:119:VAL:HG13	1.99	0.45
1:A:157:SER:O	1:A:158:LEU:C	2.58	0.45
1:B:230:PRO:HD2	1:B:233:LEU:HD22	1.99	0.45
1:A:375:GLN:O	1:A:378:VAL:HG12	2.16	0.45
1:B:72:THR:HG23	1:B:183:LYS:HB2	1.98	0.45
1:B:72:THR:HG23	1:B:183:LYS:CA	2.47	0.45
1:B:168:ASP:CG	1:B:170:ASP:HB2	2.42	0.44
1:B:28:LEU:HD22	1:B:127:ALA:HB3	1.99	0.44
1:A:54:GLU:HA	1:A:59:ASN:O	2.18	0.44
1:A:209:ILE:HG12	1:A:326:VAL:HG13	1.99	0.44
1:A:29:SER:O	1:A:31:THR:HG23	2.18	0.44
1:A:72:THR:CG2	1:A:183:LYS:CB	2.80	0.44
1:B:162:MET:HE1	1:B:172:LEU:HD22	1.99	0.44
1:A:48:ALA:CB	1:A:103:GLN:HB2	2.48	0.44
1:A:307:ILE:O	1:A:308:ALA:C	2.60	0.43
1:B:50:LEU:HD13	1:B:62:GLY:HA3	2.00	0.43
1:B:215:VAL:CG1	1:B:317:THR:HB	2.48	0.43
1:A:41:VAL:HG21	1:A:80:LEU:HD11	1.99	0.43
1:A:79:HIS:O	1:A:91:GLY:CA	2.66	0.43
1:B:80:LEU:HG	1:B:120:ALA:HB1	2.00	0.43
1:B:238:MET:HB2	1:B:276:PRO:HG2	1.99	0.43
1:A:332:VAL:CG1	1:A:368:GLY:HA3	2.49	0.43
1:B:223:ALA:HA	1:B:275:ILE:O	2.19	0.43
1:A:290:ALA:O	1:A:291:GLU:C	2.62	0.43
1:A:130:ARG:O	1:A:130:ARG:HG3	2.18	0.42
1:B:76:VAL:O	1:B:118:VAL:HA	2.18	0.42
1:B:133:MET:HE2	1:B:360:GLN:HB2	2.02	0.42
1:A:101:VAL:HG13	1:A:399:TYR:CD1	2.55	0.42
1:A:129:PHE:O	1:A:130:ARG:HG2	2.19	0.42
1:A:137:ARG:HG3	1:A:360:GLN:CG	2.50	0.42
1:A:144:PRO:HA	1:A:145:PRO:HD3	1.94	0.42
1:B:26:THR:HG23	1:B:84:TYR:HA	2.02	0.42
1:B:319:ARG:HD3	1:B:322:GLU:HB2	2.02	0.42
1:A:254[A]:ARG:HD3	1:A:254[A]:ARG:HA	1.73	0.42
1:A:20:GLN:HA	1:A:21:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:MET:HG3	1:A:399:TYR:CE1	2.55	0.41
1:B:257:THR:HG22	1:B:287:ASP:CG	2.33	0.41
1:A:38:LYS:HA	1:A:41:VAL:HG22	2.02	0.41
1:A:242:ALA:HB3	1:B:246:ILE:CD1	2.50	0.41
1:B:133:MET:CE	1:B:360:GLN:HB2	2.51	0.41
1:A:106:ASN:O	1:A:108:HIS:O	2.38	0.41
1:B:28:LEU:HB2	1:B:31:THR:HG21	2.03	0.41
1:A:133:MET:O	1:A:137:ARG:HB2	2.21	0.41
1:B:8:TRP:CE3	1:B:388:LYS:HA	2.56	0.41
1:B:212:LEU:N	1:B:293:ARG:NH1	2.68	0.41
1:B:336:ALA:HA	1:B:401:THR:OG1	2.20	0.41
1:A:236:ASP:HA	1:A:237:PRO:HD3	1.96	0.41
1:A:293:ARG:HG3	1:A:294:ASP:H	1.84	0.41
1:A:361:LEU:HD13	1:A:361:LEU:HA	1.95	0.41
1:A:130:ARG:O	1:A:130:ARG:CG	2.69	0.40
1:A:154:GLU:N	1:A:154:GLU:CD	2.79	0.40
1:A:202:PRO:HD3	5:A:434:HOH:O	2.21	0.40
1:B:278:ARG:HD2	1:B:280:GLU:OE2	2.21	0.40
1:A:137:ARG:HG3	1:A:360:GLN:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:NH1	1:B:322:GLU:OE2[1_554]	2.15	0.05

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	408/408 (100%)	391 (96%)	16 (4%)	1 (0%)	43 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	410/408 (100%)	393 (96%)	16 (4%)	1 (0%)	43	64
All	All	818/816 (100%)	784 (96%)	32 (4%)	2 (0%)	43	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	SER
1	A	78	SER

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	295/321 (92%)	274 (93%)	21 (7%)	13	25
1	B	305/321 (95%)	280 (92%)	25 (8%)	10	20
All	All	600/642 (94%)	554 (92%)	46 (8%)	12	22

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	67	THR
1	A	72	THR
1	A	92	PRO
1	A	119	VAL
1	A	130	ARG
1	A	146	GLU
1	A	154	GLU
1	A	170	ASP
1	A	190	ILE
1	A	205	ILE
1	A	244	ILE
1	A	254[A]	ARG
1	A	254[B]	ARG

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Mol	Chain	Res	Type
1	A	265	LEU
1	A	315	VAL
1	A	321	GLN
1	A	326	VAL
1	A	350	LEU
1	A	361	LEU
1	A	372	VAL
1	B	25	VAL
1	B	34	GLU
1	B	72	THR
1	B	107	GLU
1	B	122	THR
1	B	172	LEU
1	B	178	LYS
1	B	212	LEU
1	B	222	LYS
1	B	233	LEU
1	B	257	THR
1	B	286	ARG
1	B	295	GLN
1	B	306	THR
1	B	315	VAL
1	B	318[A]	GLU
1	B	318[B]	GLU
1	B	350	LEU
1	B	360	GLN
1	B	361	LEU
1	B	364	ILE
1	B	371	PHE
1	B	374	SER
1	B	389	GLU
1	B	404	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	A	400	HIS
1	B	192	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IPA	A	409	-	3,3,3	0.55	0	3,3,3	0.21	0
4	CAC	B	410	-	2,4,4	2.91	2 (100%)	4,6,6	1.73	1 (25%)
2	IPA	B	409	-	3,3,3	0.61	0	3,3,3	0.18	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	410	CAC	AS-C1	2.98	1.97	1.90
4	B	410	CAC	AS-C2	2.83	1.97	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	410	CAC	O2-AS-C2	2.33	111.48	105.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	406/408 (99%)	-0.28	6 (1%) 72 71	4, 16, 43, 49	4 (0%)
1	B	406/408 (99%)	-0.59	0 100 100	2, 10, 21, 28	6 (1%)
All	All	812/816 (99%)	-0.43	6 (0%) 84 84	2, 13, 37, 49	10 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	PRO	3.3
1	A	156	ILE	2.4
1	A	130	ARG	2.3
1	A	22	SER	2.2
1	A	178	LYS	2.2
1	A	23	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CAC	B	410	5/5	0.75	0.29	100,100,100,102	0
2	IPA	B	409	4/4	0.81	0.22	37,37,37,38	0
2	IPA	A	409	4/4	0.89	0.12	17,18,18,18	0
3	CO	B	411	1/1	0.99	0.02	9,9,9,9	0
3	CO	A	410	1/1	0.99	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.