



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 AM UTC

PDB ID : 3BLS / pdb_00003bls
Title : AMPC BETA-LACTAMASE FROM ESCHERICHIA COLI
Authors : Usher, K.C.; Shoichet, B.K.; Remington, S.J.
Deposited on : 1998-06-04
Resolution : 2.30 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

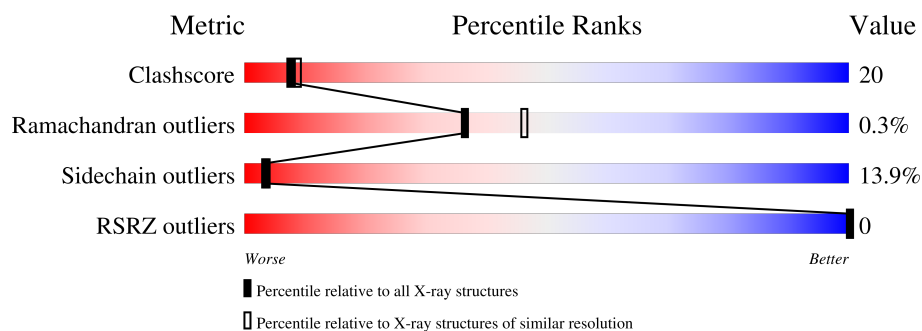
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	358	
1	B	358	

2 Entry composition [i](#)

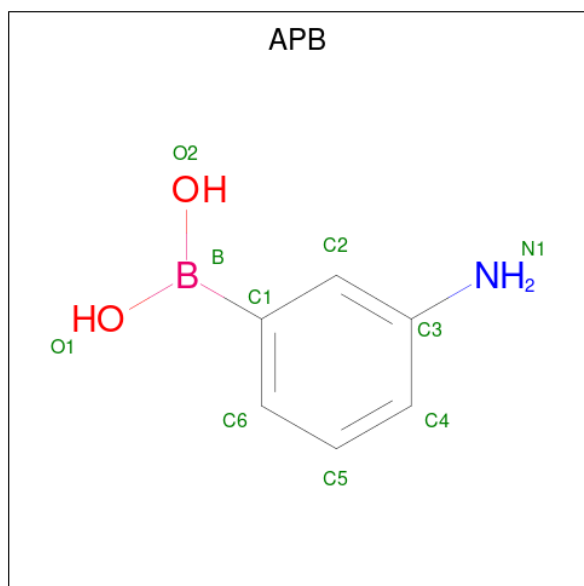
There are 3 unique types of molecules in this entry. The entry contains 5707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AMPC BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	16	0	0
			2790	1799	474	511	6			
1	B	357	Total	C	N	O	S	13	0	0
			2790	1799	474	511	6			

- Molecule 2 is M-AMINOPHENYLBORONIC ACID (CCD ID: APB) (formula: C₆H₈BNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			10	1	6	1	2		
2	B	1	Total	B	C	N	O	0	0
			10	1	6	1	2		

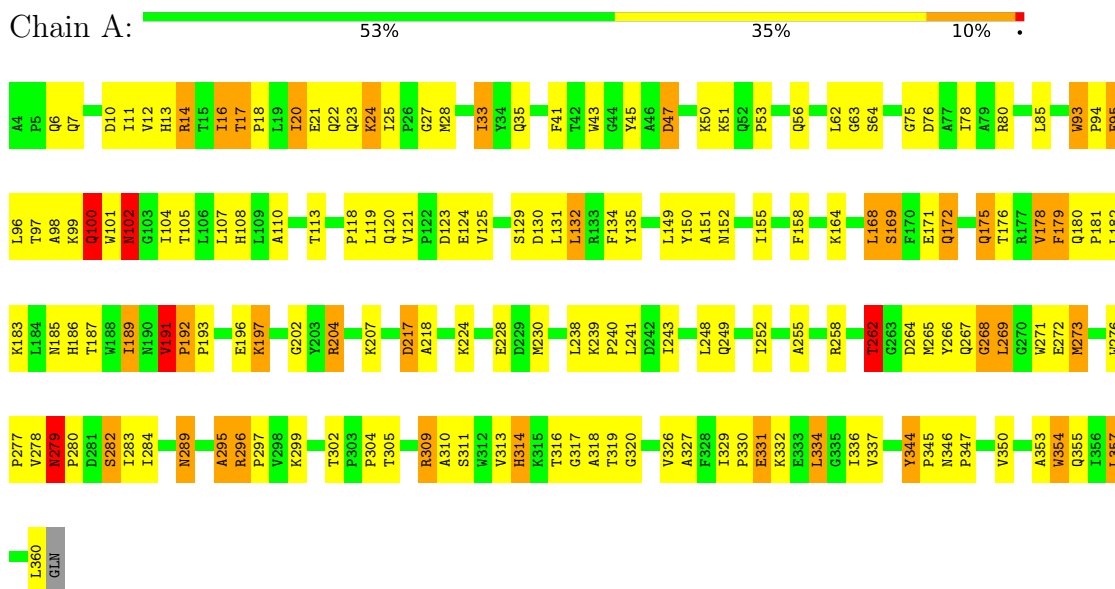
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	50	Total 50	O 50	0	0

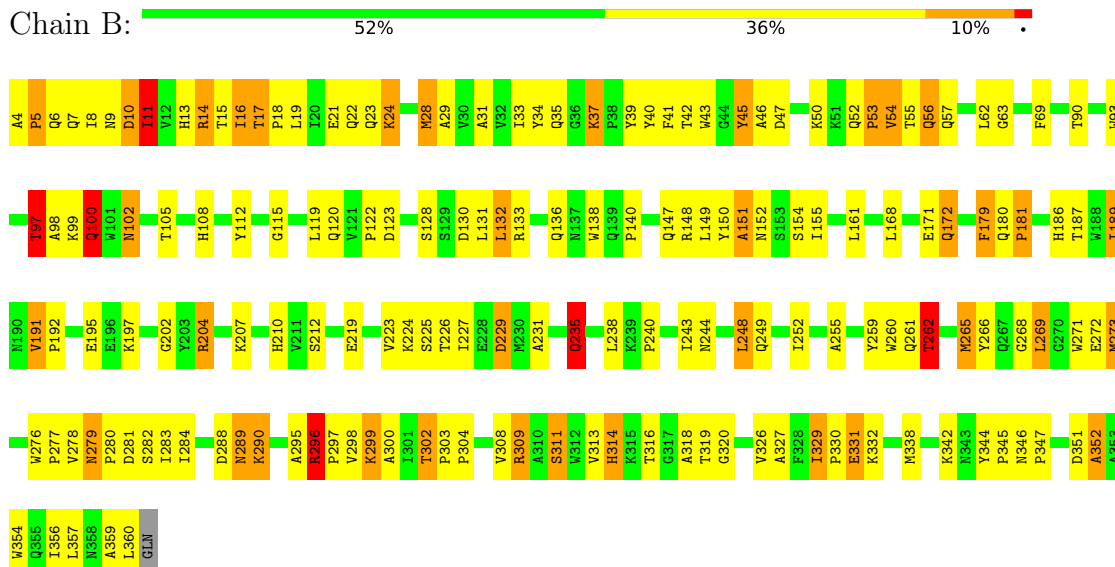
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: AMPC BETA-LACTAMASE



• Molecule 1: AMPC BETA-LACTAMASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.38Å 78.97Å 99.30Å 90.00° 116.30° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (25.00-2.30) 95.3 (25.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	136.72 (at 1.96Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.159 , (Not available) 0.149 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 102.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5707	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: APB

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	1.57	11/2870 (0.4%)	1.80	45/3921 (1.1%)
1	B	1.51	11/2870 (0.4%)	1.85	54/3921 (1.4%)
All	All	1.54	22/5740 (0.4%)	1.83	99/7842 (1.3%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	SER	CA-C	-8.55	1.42	1.52
1	B	261	GLN	N-CA	-7.52	1.36	1.46
1	A	12	VAL	CA-C	-7.19	1.44	1.52
1	B	311	SER	CA-C	-6.76	1.44	1.52
1	B	11	ILE	CA-C	-6.51	1.45	1.52
1	A	295	ALA	CA-C	-6.17	1.44	1.52
1	A	47	ASP	CA-C	-6.15	1.46	1.53
1	A	25	ILE	CA-C	-6.09	1.48	1.53
1	A	336	ILE	N-CA	-6.07	1.39	1.46
1	B	151	ALA	CA-C	6.07	1.59	1.52
1	A	47	ASP	N-CA	-5.92	1.39	1.46
1	A	337	VAL	C-O	-5.90	1.18	1.24
1	A	178	VAL	C-N	-5.78	1.26	1.33
1	B	352	ALA	N-CA	-5.69	1.39	1.46
1	A	28	MET	N-CA	-5.34	1.39	1.46
1	B	53	PRO	C-N	-5.30	1.27	1.33
1	B	45	TYR	N-CA	-5.22	1.39	1.45
1	B	342	LYS	N-CA	-5.13	1.40	1.46
1	B	10	ASP	CG-OD1	5.12	1.35	1.25
1	B	13	HIS	CG-ND1	5.08	1.43	1.38
1	B	34	TYR	N-CA	-5.05	1.40	1.46
1	A	155	ILE	N-CA	-5.01	1.40	1.46

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	HIS	CA-CB-CG	-8.86	104.94	113.80
1	B	189	ILE	N-CA-C	-8.39	104.35	111.56
1	B	56	GLN	CA-CB-CG	-8.13	97.83	114.10
1	B	17	THR	CA-C-O	7.77	125.75	118.44
1	A	27	GLY	O-C-N	-7.67	116.53	123.36
1	A	13	HIS	CA-CB-CG	-7.67	106.13	113.80
1	A	262	THR	CB-CA-C	-7.63	99.10	110.24
1	A	279	ASN	CA-C-O	7.56	124.21	119.29
1	B	97	THR	N-CA-CB	-7.50	98.73	110.44
1	A	189	ILE	N-CA-C	-7.49	104.48	111.45
1	B	316	THR	CA-CB-OG1	-7.14	98.89	109.60
1	B	16	ILE	N-CA-C	7.13	117.21	110.30
1	B	130	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	229	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	289	ASN	CA-CB-CG	-6.83	105.77	112.60
1	A	202	GLY	N-CA-C	-6.81	103.42	112.82
1	B	115	GLY	CA-C-N	-6.77	113.29	122.63
1	B	115	GLY	C-N-CA	-6.77	113.29	122.63
1	B	289	ASN	N-CA-C	6.66	119.11	111.11
1	B	97	THR	N-CA-C	6.64	121.46	113.23
1	B	224	LYS	N-CA-CB	6.39	122.01	111.08
1	B	31	ALA	CA-C-N	-6.24	115.06	123.10
1	B	31	ALA	C-N-CA	-6.24	115.06	123.10
1	B	223	VAL	N-CA-C	6.21	118.31	108.87
1	B	93	TRP	CA-C-N	6.17	125.85	119.56
1	B	93	TRP	C-N-CA	6.17	125.85	119.56
1	A	53	PRO	CB-CA-C	-6.13	102.14	110.60
1	A	113	THR	CA-CB-OG1	-6.12	100.42	109.60
1	B	5	PRO	N-CA-CB	6.11	108.62	103.25
1	A	20	ILE	CA-C-O	6.10	127.30	120.95
1	A	121	VAL	N-CA-CB	6.08	116.74	110.23
1	A	93	TRP	CA-C-N	6.03	127.38	119.84
1	A	93	TRP	C-N-CA	6.03	127.38	119.84
1	A	179	PHE	CA-CB-CG	-6.03	107.78	113.80
1	A	33	ILE	N-CA-CB	6.02	118.94	111.41
1	A	310	ALA	CA-C-N	-6.02	112.46	122.21
1	A	310	ALA	C-N-CA	-6.02	112.46	122.21
1	B	300	ALA	CA-C-N	-6.02	114.93	123.11
1	B	300	ALA	C-N-CA	-6.02	114.93	123.11
1	A	100	GLN	CB-CA-C	-5.99	101.22	110.81
1	B	154	SER	CA-C-O	5.95	127.04	120.80
1	B	319	THR	CA-CB-CG2	-5.92	100.43	110.50
1	A	217	ASP	CA-C-N	-5.87	112.61	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ASP	C-N-CA	-5.87	112.61	120.54
1	B	304	PRO	N-CA-CB	5.86	108.45	103.35
1	B	319	THR	N-CA-C	-5.85	101.26	109.69
1	A	305	THR	CA-C-O	5.83	124.44	119.66
1	A	311	SER	O-C-N	5.83	130.23	123.17
1	A	16	ILE	N-CA-C	5.77	115.95	110.53
1	A	192	PRO	CA-C-N	5.76	125.23	119.24
1	A	192	PRO	C-N-CA	5.76	125.23	119.24
1	A	135	TYR	N-CA-C	5.64	117.23	111.14
1	B	69	PHE	CA-CB-CG	-5.61	108.19	113.80
1	B	122	PRO	N-CA-CB	5.59	108.22	103.19
1	B	308	VAL	N-CA-CB	-5.58	104.70	110.95
1	B	262	THR	CB-CA-C	-5.58	101.22	110.14
1	B	161	LEU	N-CA-C	5.56	117.42	111.36
1	B	33	ILE	N-CA-CB	5.55	118.67	111.67
1	A	268	GLY	N-CA-C	-5.53	102.82	112.55
1	B	314	HIS	N-CA-C	5.53	115.68	107.88
1	B	37	LYS	CB-CA-C	5.51	116.31	108.76
1	B	56	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	A	334	LEU	N-CA-CB	-5.49	101.39	111.37
1	A	319	THR	N-CA-C	-5.48	101.80	109.69
1	B	46	ALA	CA-C-O	5.44	125.97	119.60
1	B	15	THR	N-CA-C	5.42	118.02	111.40
1	A	334	LEU	CB-CA-C	-5.41	98.07	109.38
1	B	130	ASP	N-CA-C	-5.41	105.38	111.28
1	B	172	GLN	N-CA-CB	5.39	118.04	110.12
1	B	224	LYS	CA-C-N	-5.38	113.17	122.10
1	B	224	LYS	C-N-CA	-5.38	113.17	122.10
1	B	202	GLY	CA-C-N	-5.38	115.22	122.86
1	B	202	GLY	C-N-CA	-5.38	115.22	122.86
1	A	314	HIS	N-CA-C	5.34	116.39	108.60
1	B	11	ILE	CB-CA-C	-5.33	104.88	111.70
1	A	191	VAL	N-CA-CB	5.31	118.64	111.21
1	A	175	GLN	CB-CA-C	-5.30	102.80	110.96
1	A	316	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	187	THR	CB-CA-C	5.28	118.93	110.16
1	A	304	PRO	N-CA-CB	5.25	107.92	103.35
1	B	338	MET	CA-CB-CG	-5.25	103.61	114.10
1	B	235	GLN	N-CA-CB	5.18	117.74	110.12
1	A	45	TYR	N-CA-C	5.16	118.15	109.95
1	A	102	ASN	N-CA-CB	5.15	119.20	110.49
1	B	354	TRP	CA-C-O	5.14	125.87	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	PRO	CA-C-N	-5.11	114.11	122.54
1	B	181	PRO	C-N-CA	-5.11	114.11	122.54
1	B	179	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	344	TYR	CA-C-N	5.09	125.00	119.76
1	A	344	TYR	C-N-CA	5.09	125.00	119.76
1	A	239	LYS	O-C-N	5.06	125.45	121.20
1	B	296	ARG	CA-C-N	5.04	124.95	119.76
1	B	296	ARG	C-N-CA	5.04	124.95	119.76
1	A	186	HIS	O-C-N	5.04	128.94	122.19
1	A	134	PHE	CA-CB-CG	-5.04	108.76	113.80
1	B	100	GLN	N-CA-CB	5.04	118.75	110.39
1	A	169	SER	N-CA-C	-5.03	103.77	110.55
1	A	20	ILE	CB-CA-C	-5.02	105.37	112.14
1	B	187	THR	CB-CA-C	5.01	118.38	109.72

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	2790	0	2769	105	0
1	B	2790	0	2769	118	0
2	A	10	0	8	1	0
2	B	10	0	8	3	0
3	A	57	0	0	2	0
3	B	50	0	0	2	0
All	All	5707	0	5554	223	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 20.

All (223) 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:11:ILE:HD11	1:B:360:LEU:HD21	1.39	1.03
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.34	0.92
1:B:120:GLN:HE22	1:B:152:ASN:HD22	1.22	0.88
1:B:120:GLN:NE2	1:B:152:ASN:HD22	1.72	0.87
1:A:265:MET:HE3	1:A:272:GLU:HB3	1.56	0.87
1:B:240:PRO:HA	1:B:243:ILE:HD12	1.57	0.86
1:A:255:ALA:HA	1:A:269:LEU:HB2	1.59	0.83
1:B:11:ILE:CD1	1:B:360:LEU:HD21	2.10	0.81
1:A:240:PRO:HA	1:A:243:ILE:CD1	2.11	0.80
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.46	0.80
1:A:240:PRO:HA	1:A:243:ILE:HD12	1.65	0.79
1:A:169:SER:OG	1:A:172:GLN:HG3	1.82	0.78
1:B:238:LEU:HD23	1:B:330:PRO:HA	1.65	0.77
1:B:280:PRO:O	1:B:284:ILE:HG13	1.86	0.76
1:A:76:ASP:O	1:A:80:ARG:HG3	1.87	0.74
1:B:105:THR:H	1:B:108:HIS:CD2	2.07	0.73
1:B:105:THR:H	1:B:108:HIS:HD2	1.36	0.72
1:B:262:THR:HG23	1:B:297:PRO:O	1.90	0.72
1:A:64:SER:HB2	1:A:317:GLY:HA2	1.72	0.71
1:A:278:VAL:O	1:A:280:PRO:HD3	1.91	0.70
1:B:120:GLN:HE22	1:B:152:ASN:ND2	1.89	0.70
1:A:120:GLN:HE22	1:A:152:ASN:HD22	1.39	0.69
1:A:238:LEU:HD23	1:A:330:PRO:HA	1.74	0.68
1:B:279:ASN:OD1	1:B:282:SER:HB2	1.92	0.68
1:A:11:ILE:CD1	1:A:360:LEU:HD21	2.24	0.68
1:B:268:GLY:HA3	1:B:273:MET:HE1	1.76	0.68
1:B:16:ILE:O	1:B:19:LEU:HB3	1.93	0.67
1:B:295:ALA:O	1:B:296:ARG:HD3	1.94	0.67
1:A:11:ILE:HD12	1:A:360:LEU:HD21	1.75	0.67
1:B:97:THR:HG22	1:B:136:GLN:HE22	1.59	0.67
1:A:75:GLY:HA2	1:A:78:ILE:HD12	1.77	0.67
1:A:105:THR:H	1:A:108:HIS:CD2	2.13	0.66
1:A:265:MET:HE3	1:A:272:GLU:CB	2.26	0.66
1:A:280:PRO:O	1:A:284:ILE:HG13	1.96	0.66
1:A:171:GLU:O	1:A:175:GLN:HG3	1.96	0.65
1:A:172:GLN:O	1:A:176:THR:HG23	1.96	0.65
1:A:344:TYR:HB2	1:A:345:PRO:HD2	1.77	0.65
1:B:265:MET:HE1	1:B:272:GLU:HG2	1.76	0.65
1:A:265:MET:HG2	1:A:266:TYR:N	2.12	0.65
1:B:279:ASN:HD21	1:B:281:ASP:HB2	1.61	0.64
1:A:120:GLN:NE2	1:A:152:ASN:HD22	1.95	0.64
1:B:7:GLN:O	1:B:11:ILE:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ALA:O	1:B:235:GLN:HG3	1.98	0.63
1:A:47:ASP:OD2	1:A:50:LYS:NZ	2.29	0.63
1:B:344:TYR:HB2	1:B:345:PRO:HD2	1.80	0.63
1:B:309:ARG:NH1	1:B:331:GLU:HA	2.14	0.63
1:A:98:ALA:HB1	1:A:100:GLN:OE1	1.99	0.63
1:B:180:GLN:N	1:B:181:PRO:HD2	2.13	0.63
1:B:346:ASN:HB2	1:B:347:PRO:HD3	1.81	0.62
1:A:217:ASP:O	1:A:218:ALA:C	2.39	0.62
1:A:279:ASN:O	1:A:282:SER:HB2	2.01	0.61
1:A:295:ALA:O	1:A:296:ARG:HD3	2.00	0.61
1:A:56:GLN:NE2	1:A:228:GLU:OE2	2.36	0.59
1:B:255:ALA:HA	1:B:269:LEU:HB2	1.85	0.59
1:B:52:GLN:CD	1:B:53:PRO:HD2	2.28	0.59
1:B:240:PRO:HA	1:B:243:ILE:CD1	2.30	0.59
1:A:120:GLN:HE22	1:A:152:ASN:ND2	2.00	0.59
1:B:19:LEU:O	1:B:19:LEU:HD12	2.02	0.59
1:A:93:TRP:CZ2	1:A:132:LEU:HB2	2.39	0.58
1:A:240:PRO:CA	1:A:243:ILE:HD12	2.33	0.58
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.39	0.58
1:A:185:ASN:HB2	3:A:416:HOH:O	2.03	0.58
1:A:262:THR:HG23	1:A:297:PRO:O	2.04	0.58
1:B:288:ASP:OD1	1:B:290:LYS:HG2	2.04	0.57
1:B:11:ILE:CD1	1:B:360:LEU:HD11	2.35	0.57
1:B:120:GLN:NE2	1:B:152:ASN:ND2	2.47	0.57
1:A:6:GLN:O	1:A:7:GLN:C	2.47	0.57
1:A:17:THR:HB	1:A:18:PRO:HD3	1.87	0.57
1:A:296:ARG:HG3	1:A:296:ARG:NH1	2.11	0.56
1:B:4:ALA:HB2	1:B:39:TYR:CD2	2.41	0.55
1:B:204:ARG:HB2	1:B:320:GLY:O	2.06	0.55
1:B:240:PRO:O	1:B:249:GLN:HG3	2.07	0.55
1:B:90:THR:HG23	3:B:378:HOH:O	2.07	0.54
1:A:224:LYS:HD2	1:A:224:LYS:N	2.22	0.54
1:B:271:TRP:C	1:B:273:MET:HE3	2.32	0.54
1:A:105:THR:H	1:A:108:HIS:HD2	1.53	0.54
1:A:280:PRO:HG3	1:A:354:TRP:CH2	2.42	0.54
1:A:280:PRO:HG3	1:A:354:TRP:CZ2	2.43	0.54
1:B:260:TRP:O	1:B:266:TYR:HA	2.07	0.54
1:A:104:ILE:HA	1:A:108:HIS:HD2	1.73	0.54
1:B:192:PRO:HD2	1:B:195:GLU:HB2	1.89	0.54
1:B:186:HIS:N	1:B:229:ASP:OD2	2.39	0.53
1:B:313:VAL:O	1:B:327:ALA:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:MET:CE	1:B:272:GLU:HG2	2.38	0.53
1:B:318:ALA:N	2:B:362:APB:H2	2.23	0.53
1:B:11:ILE:HD12	1:B:360:LEU:HD11	1.91	0.53
1:A:329:ILE:O	1:A:330:PRO:C	2.50	0.53
1:B:55:THR:C	1:B:57:GLN:H	2.15	0.52
1:B:243:ILE:HD13	1:B:252:ILE:HD12	1.90	0.52
1:B:119:LEU:HA	1:B:151:ALA:HA	1.92	0.52
1:B:240:PRO:CA	1:B:243:ILE:HD12	2.34	0.52
1:B:98:ALA:HB1	1:B:100:GLN:OE1	2.10	0.52
1:B:45:TYR:HA	1:B:53:PRO:HA	1.90	0.52
1:A:240:PRO:O	1:A:243:ILE:HD12	2.09	0.52
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.45	0.52
1:B:42:THR:HB	1:B:54:VAL:HG12	1.92	0.51
1:B:148:ARG:HB2	1:B:298:VAL:HG11	1.91	0.51
1:A:193:PRO:HA	1:A:196:GLU:HG3	1.93	0.51
1:A:240:PRO:C	1:A:243:ILE:HD12	2.35	0.51
1:A:353:ALA:O	1:A:357:LEU:HB2	2.11	0.51
1:A:265:MET:HE3	1:A:272:GLU:CG	2.41	0.51
1:B:4:ALA:HB2	1:B:39:TYR:HD2	1.74	0.50
1:A:125:VAL:HG13	1:A:130:ASP:HB3	1.92	0.50
1:A:217:ASP:OD1	1:A:218:ALA:N	2.43	0.50
1:B:219:GLU:OE1	1:B:219:GLU:N	2.36	0.50
1:A:296:ARG:HH11	1:A:296:ARG:CG	2.14	0.50
1:A:355:GLN:OE1	1:A:355:GLN:HA	2.10	0.50
1:B:41:PHE:HB2	1:B:43:TRP:CZ3	2.48	0.49
1:A:175:GLN:HB3	1:A:180:GLN:NE2	2.27	0.49
1:B:243:ILE:CD1	1:B:252:ILE:HD12	2.43	0.49
1:B:23:GLN:O	1:B:24:LYS:HB2	2.12	0.49
1:B:29:ALA:C	1:B:227:ILE:HD13	2.38	0.48
1:B:352:ALA:O	1:B:356:ILE:HG13	2.12	0.48
1:A:264:ASP:OD1	1:A:264:ASP:N	2.36	0.48
1:B:171:GLU:HG3	1:B:189:ILE:HB	1.95	0.48
1:A:243:ILE:HD13	1:A:252:ILE:HD12	1.95	0.48
1:A:318:ALA:N	2:A:362:APB:H2	2.28	0.48
1:A:100:GLN:C	1:A:102:ASN:H	2.22	0.48
1:A:279:ASN:ND2	1:A:282:SER:H	2.12	0.48
1:B:259:TYR:CE1	1:B:269:LEU:HD13	2.48	0.48
1:B:296:ARG:HG3	1:B:296:ARG:NH1	2.21	0.48
1:B:344:TYR:HB2	1:B:345:PRO:CD	2.43	0.48
1:A:265:MET:CE	1:A:272:GLU:HG2	2.44	0.48
1:B:41:PHE:HB3	1:B:43:TRP:CH2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:O	1:B:329:ILE:HG23	2.14	0.47
1:A:10:ASP:O	1:A:14:ARG:HB2	2.14	0.47
1:A:179:PHE:N	1:A:179:PHE:CD1	2.79	0.47
1:B:238:LEU:CD2	1:B:330:PRO:HA	2.40	0.47
1:A:80:ARG:HH11	1:A:80:ARG:HD3	1.52	0.47
1:B:17:THR:N	1:B:18:PRO:HD2	2.30	0.47
1:B:100:GLN:OE1	1:B:100:GLN:N	2.29	0.47
1:B:100:GLN:H	1:B:100:GLN:CD	2.19	0.47
1:A:197:LYS:HD2	3:A:395:HOH:O	2.14	0.47
1:B:8:ILE:O	1:B:9:ASN:C	2.54	0.47
1:B:19:LEU:HD12	1:B:19:LEU:C	2.38	0.47
1:A:119:LEU:HA	1:A:151:ALA:HA	1.96	0.47
1:A:149:LEU:O	1:A:150:TYR:C	2.58	0.47
1:A:118:PRO:O	1:A:151:ALA:HB1	2.15	0.46
1:B:346:ASN:N	1:B:347:PRO:CD	2.77	0.46
1:A:85:LEU:HB3	1:A:107:LEU:HB2	1.96	0.46
1:A:346:ASN:N	1:A:347:PRO:CD	2.79	0.46
1:A:278:VAL:HG22	1:A:279:ASN:N	2.30	0.46
1:B:302:THR:HA	1:B:303:PRO:HA	1.75	0.46
1:A:344:TYR:HB2	1:A:345:PRO:CD	2.44	0.46
1:B:4:ALA:CB	1:B:39:TYR:CD2	2.99	0.45
1:B:10:ASP:HB3	1:B:14:ARG:NH1	2.31	0.45
1:B:41:PHE:CB	1:B:43:TRP:CH2	3.00	0.45
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.61	0.45
1:A:171:GLU:HG3	1:A:189:ILE:HD12	1.99	0.45
1:B:289:ASN:HD22	1:B:289:ASN:HA	1.42	0.45
1:A:309:ARG:NH1	1:A:331:GLU:HA	2.32	0.45
1:A:17:THR:N	1:A:18:PRO:HD2	2.32	0.44
1:B:56:GLN:HG3	3:B:366:HOH:O	2.17	0.44
1:B:191:VAL:HA	1:B:192:PRO:HD3	1.86	0.44
1:B:225:SER:OG	1:B:226:THR:N	2.49	0.44
1:A:182:LEU:O	1:A:183:LYS:HB2	2.17	0.44
1:B:309:ARG:O	1:B:331:GLU:HB3	2.17	0.44
1:A:110:ALA:HB2	1:A:158:PHE:CD1	2.53	0.44
1:A:204:ARG:NH1	1:A:204:ARG:HG3	2.31	0.44
1:A:271:TRP:HB3	1:A:273:MET:HE2	2.00	0.44
1:B:62:LEU:O	1:B:63:GLY:C	2.60	0.44
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.87	0.44
1:B:39:TYR:CD1	1:B:39:TYR:N	2.86	0.43
1:A:101:TRP:O	1:A:102:ASN:C	2.60	0.43
1:A:204:ARG:HB2	1:A:320:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TRP:CH2	1:B:140:PRO:HB3	2.53	0.43
1:B:41:PHE:CD1	1:B:41:PHE:N	2.86	0.43
1:B:6:GLN:O	1:B:7:GLN:C	2.62	0.43
1:B:131:LEU:HD12	1:B:131:LEU:HA	1.72	0.43
1:A:271:TRP:CB	1:A:273:MET:CE	2.97	0.43
1:A:313:VAL:O	1:A:327:ALA:HA	2.19	0.43
1:B:5:PRO:O	1:B:6:GLN:C	2.61	0.43
1:B:47:ASP:OD2	1:B:50:LYS:NZ	2.36	0.43
1:B:52:GLN:HA	1:B:52:GLN:NE2	2.33	0.43
1:B:150:TYR:CE2	2:B:362:APB:H6	2.54	0.43
1:B:318:ALA:HB2	2:B:362:APB:HN11	1.83	0.43
1:B:17:THR:HB	1:B:18:PRO:HD3	2.01	0.43
1:B:299:LYS:HE3	1:B:299:LYS:HB2	1.71	0.43
1:B:6:GLN:HA	1:B:9:ASN:HB2	2.00	0.42
1:B:279:ASN:ND2	1:B:281:ASP:HB2	2.31	0.42
1:B:52:GLN:OE1	1:B:53:PRO:HD2	2.18	0.42
1:A:41:PHE:HB2	1:A:43:TRP:CZ3	2.53	0.42
1:A:191:VAL:HA	1:A:192:PRO:HD3	1.76	0.42
1:A:204:ARG:HH11	1:A:204:ARG:CG	2.33	0.42
1:A:278:VAL:CG2	1:A:279:ASN:N	2.82	0.42
1:B:123:ASP:OD1	1:B:123:ASP:N	2.52	0.42
1:A:180:GLN:N	1:A:181:PRO:CD	2.81	0.42
1:B:41:PHE:CB	1:B:43:TRP:CZ3	3.02	0.42
1:B:112:TYR:HB3	1:B:149:LEU:O	2.20	0.42
1:B:271:TRP:HB2	1:B:273:MET:CE	2.49	0.42
1:B:240:PRO:O	1:B:243:ILE:HD12	2.19	0.42
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.77	0.42
1:B:40:TYR:C	1:B:41:PHE:CD1	2.98	0.42
1:B:171:GLU:HG3	1:B:189:ILE:HD12	2.01	0.42
1:B:351:ASP:O	1:B:352:ALA:C	2.61	0.42
1:B:271:TRP:CB	1:B:273:MET:CE	2.98	0.42
1:B:359:ALA:C	1:B:360:LEU:HG	2.43	0.42
1:A:33:ILE:O	1:A:334:LEU:HA	2.20	0.41
1:B:272:GLU:N	1:B:273:MET:HE3	2.35	0.41
1:A:7:GLN:O	1:A:11:ILE:HG13	2.20	0.41
1:A:23:GLN:O	1:A:24:LYS:HB2	2.21	0.41
1:A:230:MET:HE3	1:A:230:MET:HB3	1.95	0.41
1:A:94:PRO:HD2	1:A:95:GLU:OE2	2.21	0.41
1:A:240:PRO:O	1:A:249:GLN:HG3	2.19	0.41
1:B:55:THR:C	1:B:57:GLN:N	2.79	0.41
1:A:62:LEU:O	1:A:63:GLY:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TRP:O	1:A:96:LEU:HB2	2.19	0.41
1:A:258:ARG:HH11	1:A:258:ARG:HD3	1.66	0.41
1:A:267:GLN:HG3	1:A:268:GLY:O	2.21	0.41
1:A:314:HIS:HB2	1:A:326:VAL:O	2.20	0.41
1:B:278:VAL:HG22	1:B:279:ASN:N	2.34	0.41
1:A:16:ILE:HG22	1:A:20:ILE:CD1	2.51	0.41
1:A:271:TRP:HB3	1:A:273:MET:CE	2.51	0.41
1:B:179:PHE:N	1:B:179:PHE:CD1	2.84	0.41
1:A:346:ASN:O	1:A:350:VAL:HG23	2.21	0.40
1:B:314:HIS:CD2	1:B:314:HIS:C	2.99	0.40
1:B:314:HIS:HB2	1:B:326:VAL:O	2.21	0.40
1:A:168:LEU:HD22	1:A:172:GLN:NE2	2.37	0.40
1:A:178:VAL:O	1:A:179:PHE:C	2.63	0.40
1:A:289:ASN:HD22	1:A:289:ASN:HA	1.27	0.40
1:B:28:MET:HG3	1:B:29:ALA:N	2.37	0.40
1:B:132:LEU:O	1:B:133:ARG:C	2.63	0.40
1:B:56:GLN:HB2	1:B:57:GLN:NE2	2.37	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	355/358 (99%)	340 (96%)	14 (4%)	1 (0%)	36	46
1	B	355/358 (99%)	330 (93%)	24 (7%)	1 (0%)	36	46
All	All	710/716 (99%)	670 (94%)	38 (5%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	ASN

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Mol	Chain	Res	Type
1	A	102	ASN

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	291/292 (100%)	252 (87%)	39 (13%)	4	4
1	B	291/292 (100%)	249 (86%)	42 (14%)	3	3
All	All	582/584 (100%)	501 (86%)	81 (14%)	3	4

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	THR
1	A	21	GLU
1	A	22	GLN
1	A	24	LYS
1	A	35	GLN
1	A	51	LYS
1	A	95	GLU
1	A	97	THR
1	A	99	LYS
1	A	100	GLN
1	A	102	ASN
1	A	123	ASP
1	A	124	GLU
1	A	129	SER
1	A	132	LEU
1	A	164	LYS
1	A	168	LEU
1	A	172	GLN
1	A	191	VAL
1	A	197	LYS
1	A	204	ARG

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Mol	Chain	Res	Type
1	A	207	LYS
1	A	241	LEU
1	A	248	LEU
1	A	262	THR
1	A	269	LEU
1	A	273	MET
1	A	279	ASN
1	A	282	SER
1	A	283	ILE
1	A	296	ARG
1	A	299	LYS
1	A	302	THR
1	A	309	ARG
1	A	331	GLU
1	A	332	LYS
1	A	354	TRP
1	A	357	LEU
1	B	11	ILE
1	B	14	ARG
1	B	21	GLU
1	B	22	GLN
1	B	24	LYS
1	B	28	MET
1	B	35	GLN
1	B	37	LYS
1	B	54	VAL
1	B	97	THR
1	B	99	LYS
1	B	100	GLN
1	B	102	ASN
1	B	128	SER
1	B	132	LEU
1	B	147	GLN
1	B	155	ILE
1	B	168	LEU
1	B	172	GLN
1	B	191	VAL
1	B	197	LYS
1	B	204	ARG
1	B	207	LYS
1	B	212	SER
1	B	235	GLN

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Mol	Chain	Res	Type
1	B	244	ASN
1	B	248	LEU
1	B	262	THR
1	B	265	MET
1	B	269	LEU
1	B	273	MET
1	B	279	ASN
1	B	283	ILE
1	B	290	LYS
1	B	296	ARG
1	B	299	LYS
1	B	302	THR
1	B	309	ARG
1	B	329	ILE
1	B	331	GLU
1	B	332	LYS
1	B	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	52	GLN
1	A	56	GLN
1	A	102	ASN
1	A	108	HIS
1	A	120	GLN
1	A	172	GLN
1	A	180	GLN
1	A	185	ASN
1	A	190	ASN
1	A	279	ASN
1	A	289	ASN
1	B	13	HIS
1	B	23	GLN
1	B	52	GLN
1	B	56	GLN
1	B	57	GLN
1	B	108	HIS
1	B	120	GLN
1	B	137	ASN
1	B	139	GLN

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Mol	Chain	Res	Type
1	B	172	GLN
1	B	175	GLN
1	B	180	GLN
1	B	198	ASN
1	B	289	ASN
1	B	358	ASN

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](#)

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	APB	B	362	1	10,10,10	7.91	3 (30%)	13,13,13	2.08	3 (23%)
2	APB	A	362	1	10,10,10	7.69	3 (30%)	13,13,13	2.25	5 (38%)

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	APB	B	362	1	-	2/4/4/4	0/1/1/1
2	APB	A	362	1	-	2/4/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	362	APB	B-O2	18.97	1.67	1.36
2	A	362	APB	B-O2	18.81	1.67	1.36
2	B	362	APB	B-O1	14.61	1.60	1.36
2	A	362	APB	B-O1	14.57	1.60	1.36
2	B	362	APB	B-C1	7.13	1.71	1.57
2	A	362	APB	B-C1	4.99	1.67	1.57

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	362	APB	O1-B-C1	-5.42	103.63	119.96
2	A	362	APB	O2-B-C1	-4.46	106.51	119.96
2	A	362	APB	O1-B-C1	-4.16	107.41	119.96
2	B	362	APB	O2-B-C1	-3.34	109.88	119.96
2	A	362	APB	C5-C6-C1	-2.86	118.85	121.58
2	A	362	APB	O2-B-O1	-2.80	110.40	119.65
2	A	362	APB	C6-C1-C2	2.79	120.51	117.41
2	B	362	APB	O2-B-O1	-2.58	111.12	119.65

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	362	APB	O2-B-C1-C2
2	A	362	APB	O2-B-C1-C6
2	B	362	APB	O2-B-C1-C2
2	B	362	APB	O2-B-C1-C6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	362	APB	3	0
2	A	362	APB	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 [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	357/358 (99%)	-0.73	0 100 100	4, 16, 55, 77	4 (1%)
1	B	357/358 (99%)	-0.65	0 100 100	4, 17, 56, 79	4 (1%)
All	All	714/716 (99%)	-0.69	0 100 100	4, 17, 56, 79	8 (1%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	APB	B	362	10/10	0.87	0.21	24,69,100,100	0
2	APB	A	362	10/10	0.89	0.17	23,68,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.