



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:52 PM UTC

PDB ID : 1BLH / pdb_00001blh
Title : STRUCTURE OF A PHOSPHONATE-INHIBITED BETA-LACTAMASE.
AN ANALOG OF THE TETRAHEDRAL TRANSITION STATE(SLASH)I
NTERMEDIATE OF BETA-LACTAM HYDROLYSIS
Authors : Chen, C.C.H.; Herzberg, O.
Deposited on : 1993-09-30
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)
Xtrriage (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

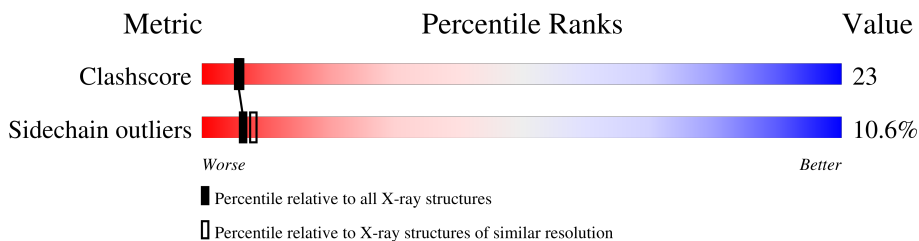
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)
Sidechain outliers	187428	6854 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	257	

2 Entry composition [i](#)

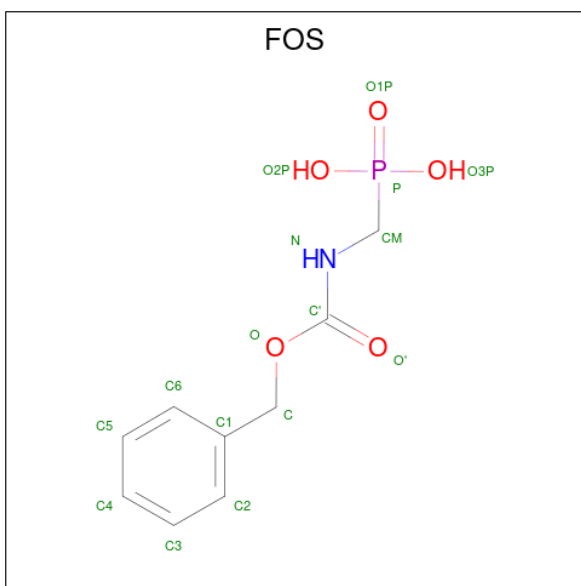
There are 3 unique types of molecules in this entry. The entry contains 2209 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	1999	1274	334	388	3	0	0	0

- Molecule 2 is [[N-(BENZYLOXYCARBONYL)AMINO]METHYL]PHOSPHATE (CCD ID: FOS) (formula: C₉H₁₂NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	15	9	1	4	1	0	0

- Molecule 3 is water.

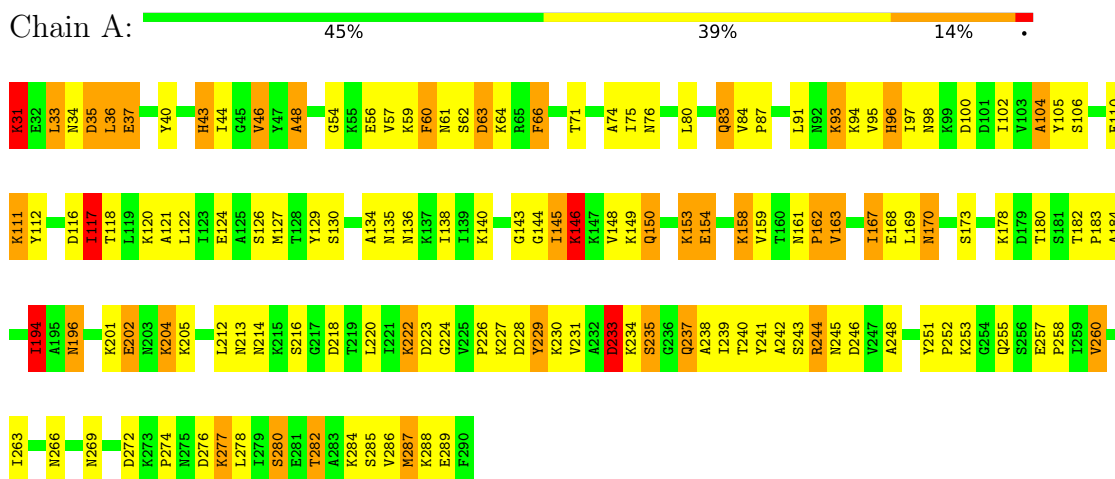
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total	O	0	0
			195	195		

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. 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. 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: BETA-LACTAMASE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	53.96Å 94.20Å 138.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2209	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: FOS

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	1.44	4/2029 (0.2%)	2.25	97/2731 (3.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	THR	CA-CB	5.61	1.63	1.53
1	A	104	ALA	N-CA	5.57	1.52	1.46
1	A	145	ILE	C-N	-5.32	1.27	1.33
1	A	228	ASP	CA-CB	5.10	1.61	1.53

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	HIS	CA-CB-CG	-10.22	103.58	113.80
1	A	145	ILE	CA-C-N	9.87	133.27	120.44
1	A	145	ILE	C-N-CA	9.87	133.27	120.44
1	A	170	ASN	CA-CB-CG	-9.11	103.50	112.60
1	A	35	ASP	CA-CB-CG	8.67	121.27	112.60
1	A	213	ASN	CA-CB-CG	-8.44	104.16	112.60
1	A	43	HIS	CA-CB-CG	-8.41	105.39	113.80
1	A	269	ASN	OD1-CG-ND2	7.62	130.22	122.60
1	A	146	LYS	N-CA-CB	-7.58	99.03	110.01
1	A	218	ASP	N-CA-C	7.50	120.33	111.71
1	A	228	ASP	N-CA-C	7.48	119.43	111.28
1	A	245	ASN	CA-CB-CG	7.30	119.90	112.60
1	A	226	PRO	CA-C-N	7.21	130.26	120.38
1	A	226	PRO	C-N-CA	7.21	130.26	120.38
1	A	143	GLY	CA-C-O	-7.20	111.75	118.95
1	A	163	VAL	CB-CA-C	7.00	117.28	111.05
1	A	117	ILE	CB-CG1-CD1	6.94	128.37	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	PHE	CA-CB-CG	6.93	120.73	113.80
1	A	214	ASN	CA-CB-CG	-6.86	105.74	112.60
1	A	95	VAL	CA-C-O	6.78	128.21	120.76
1	A	33	LEU	CB-CA-C	6.76	122.34	110.85
1	A	71	THR	N-CA-CB	6.75	120.61	110.22
1	A	194	ILE	O-C-N	6.69	126.93	121.85
1	A	135	ASN	OD1-CG-ND2	-6.64	115.95	122.60
1	A	129	TYR	O-C-N	6.55	130.17	122.24
1	A	104	ALA	N-CA-CB	-6.55	100.42	110.04
1	A	184	ALA	CA-C-O	-6.50	114.01	120.70
1	A	222	LYS	N-CA-CB	6.49	120.40	110.14
1	A	223	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	145	ILE	CA-C-O	6.37	127.39	120.57
1	A	93	LYS	CA-C-O	6.35	128.28	121.55
1	A	105	TYR	CA-C-N	6.33	129.62	122.59
1	A	105	TYR	C-N-CA	6.33	129.62	122.59
1	A	83	GLN	O-C-N	6.30	129.64	122.20
1	A	287	MET	CB-CA-C	6.30	121.25	110.79
1	A	227	LYS	CA-C-N	6.25	128.66	120.28
1	A	227	LYS	C-N-CA	6.25	128.66	120.28
1	A	93	LYS	N-CA-CB	6.22	119.18	110.04
1	A	235	SER	CA-C-N	6.19	129.44	121.27
1	A	235	SER	C-N-CA	6.19	129.44	121.27
1	A	140	LYS	O-C-N	6.17	128.76	122.09
1	A	91	LEU	CA-C-O	6.13	127.02	119.05
1	A	136	ASN	CA-C-O	-6.07	114.45	120.82
1	A	162	PRO	CB-CA-C	6.06	116.92	111.40
1	A	48	ALA	CA-C-O	6.05	127.04	120.32
1	A	158	LYS	N-CA-CB	6.01	119.34	110.56
1	A	150	GLN	CA-C-N	5.99	128.31	120.28
1	A	150	GLN	C-N-CA	5.99	128.31	120.28
1	A	240	THR	N-CA-C	5.97	119.45	109.95
1	A	173	SER	O-C-N	5.96	128.17	121.32
1	A	54	GLY	N-CA-C	-5.94	107.05	115.43
1	A	241	TYR	O-C-N	5.90	130.31	122.41
1	A	100	ASP	CB-CG-OD2	-5.89	104.84	118.40
1	A	63	ASP	CA-CB-CG	-5.87	106.73	112.60
1	A	57	VAL	N-CA-CB	5.83	119.46	111.41
1	A	71	THR	CA-C-O	-5.80	113.55	120.10
1	A	154	GLU	CA-C-O	-5.75	113.61	120.10
1	A	148	VAL	O-C-N	5.74	127.54	121.91
1	A	74	ALA	O-C-N	5.67	128.22	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	LYS	CB-CG-CD	5.67	124.35	111.30
1	A	269	ASN	O-C-N	5.62	129.93	123.29
1	A	46	VAL	CA-C-O	5.61	126.95	120.67
1	A	248	ALA	N-CA-C	5.61	117.60	109.07
1	A	36	LEU	N-CA-C	-5.59	104.81	111.69
1	A	260	VAL	O-C-N	5.54	129.03	122.83
1	A	46	VAL	CA-C-N	5.51	130.57	121.86
1	A	46	VAL	C-N-CA	5.51	130.57	121.86
1	A	205	LYS	CB-CA-C	5.50	120.76	110.70
1	A	158	LYS	CA-CB-CG	5.48	125.06	114.10
1	A	60	PHE	CB-CA-C	5.47	118.23	110.24
1	A	276	ASP	CB-CA-C	5.47	119.87	110.79
1	A	269	ASN	CB-CG-ND2	-5.42	108.28	116.40
1	A	282	THR	CA-C-N	5.40	127.78	120.65
1	A	282	THR	C-N-CA	5.40	127.78	120.65
1	A	269	ASN	CA-CB-CG	-5.36	107.24	112.60
1	A	257	GLU	CG-CD-OE2	-5.34	106.12	118.40
1	A	234	LYS	N-CA-CB	5.33	119.21	110.90
1	A	138	ILE	O-C-N	5.31	127.11	121.91
1	A	161	ASN	N-CA-CB	-5.30	102.50	111.30
1	A	288	LYS	N-CA-C	5.28	118.51	111.75
1	A	37	GLU	CA-C-O	5.26	126.34	120.82
1	A	31	LYS	CA-CB-CG	5.25	124.61	114.10
1	A	146	LYS	CB-CG-CD	5.22	123.30	111.30
1	A	95	VAL	CB-CA-C	5.20	119.70	110.71
1	A	266	ASN	CA-C-O	5.18	126.87	121.38
1	A	167	ILE	CA-C-N	5.15	127.44	120.38
1	A	167	ILE	C-N-CA	5.15	127.44	120.38
1	A	244	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	A	196	ASN	CA-C-O	-5.13	116.04	121.78
1	A	140	LYS	N-CA-CB	5.12	117.50	110.07
1	A	97	ILE	O-C-N	5.11	128.54	123.18
1	A	102	ILE	N-CA-C	5.08	115.66	109.30
1	A	43	HIS	O-C-N	5.04	128.97	123.27
1	A	76	ASN	CA-C-N	5.03	127.33	120.54
1	A	76	ASN	C-N-CA	5.03	127.33	120.54
1	A	233	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	180	THR	CA-CB-OG1	-5.00	102.09	109.60

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	1999	0	2042	94	0
2	A	15	0	10	1	0
3	A	195	0	0	20	0
All	All	2209	0	2052	95	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 23.

All (95) 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:251:TYR:HA	3:A:349:HOH:O	1.50	1.12
1:A:237:GLN:HG3	1:A:244:ARG:HD3	1.47	0.96
1:A:146:LYS:HE3	3:A:476:HOH:O	1.68	0.91
1:A:44:ILE:HD11	1:A:278:LEU:HD11	1.52	0.90
1:A:229:TYR:HE2	1:A:287:MET:HE2	1.36	0.89
1:A:202:GLU:HG3	3:A:427:HOH:O	1.79	0.81
1:A:111:LYS:HA	1:A:111:LYS:HE2	1.63	0.79
1:A:111:LYS:HD2	3:A:432:HOH:O	1.82	0.78
1:A:252:PRO:HD2	1:A:255:GLN:HB3	1.65	0.77
1:A:63:ASP:HB2	3:A:358:HOH:O	1.84	0.76
1:A:238:ALA:HB3	1:A:243:SER:HB2	1.70	0.73
1:A:111:LYS:HE2	1:A:111:LYS:CA	2.21	0.71
1:A:153:LYS:HB3	3:A:480:HOH:O	1.94	0.68
1:A:150:GLN:O	1:A:153:LYS:HG3	1.94	0.68
1:A:229:TYR:CE2	1:A:287:MET:HE2	2.26	0.67
1:A:93:LYS:HG2	1:A:94:LYS:N	2.10	0.66
1:A:120:LYS:O	1:A:124:GLU:HG3	1.95	0.66
1:A:237:GLN:HG3	1:A:244:ARG:CD	2.27	0.63
1:A:93:LYS:O	1:A:118:THR:HA	1.98	0.63
1:A:150:GLN:O	1:A:153:LYS:CG	2.49	0.61
1:A:163:VAL:HG21	1:A:178:LYS:HG2	1.82	0.61
1:A:212:LEU:HD22	1:A:230:LYS:HE2	1.81	0.61
1:A:80:LEU:O	1:A:84:VAL:HG23	2.01	0.61
1:A:144:GLY:HA3	1:A:146:LYS:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:HA	1:A:243:SER:O	2.01	0.61
1:A:253:LYS:N	3:A:473:HOH:O	2.34	0.60
1:A:263:ILE:HD13	1:A:282:THR:HG22	1.83	0.60
1:A:202:GLU:CG	3:A:427:HOH:O	2.44	0.59
1:A:229:TYR:CD1	1:A:229:TYR:N	2.71	0.58
1:A:34:ASN:ND2	1:A:60:PHE:HE1	2.02	0.58
1:A:48:ALA:O	1:A:56:GLU:HA	2.04	0.57
1:A:80:LEU:O	1:A:83:GLN:HG2	2.04	0.57
1:A:93:LYS:CB	3:A:411:HOH:O	2.52	0.57
1:A:222:LYS:HE2	1:A:231:VAL:O	2.04	0.56
1:A:48:ALA:HA	1:A:260:VAL:O	2.06	0.56
1:A:153:LYS:HG3	1:A:154:GLU:N	2.19	0.56
1:A:31:LYS:N	1:A:31:LYS:HD2	2.21	0.55
1:A:238:ALA:HB3	1:A:243:SER:CB	2.37	0.55
1:A:159:VAL:HG11	1:A:182:THR:HG23	1.87	0.55
1:A:169:LEU:HD12	1:A:169:LEU:C	2.31	0.55
1:A:34:ASN:ND2	1:A:60:PHE:CE1	2.75	0.55
1:A:34:ASN:O	1:A:37:GLU:HB2	2.07	0.55
1:A:64:LYS:O	1:A:183:PRO:HD3	2.06	0.55
1:A:149:LYS:HD3	3:A:460:HOH:O	2.06	0.55
1:A:282:THR:O	1:A:286:VAL:HG23	2.07	0.54
1:A:202:GLU:H	1:A:202:GLU:CD	2.15	0.54
1:A:120:LYS:O	1:A:124:GLU:CG	2.56	0.54
1:A:121:ALA:HA	1:A:124:GLU:HG3	1.88	0.54
1:A:93:LYS:HB2	3:A:411:HOH:O	2.06	0.54
1:A:229:TYR:N	1:A:229:TYR:HD1	2.05	0.54
1:A:163:VAL:HG11	1:A:178:LYS:HD2	1.88	0.53
2:A:291:FOS:HM2	3:A:451:HOH:O	2.08	0.53
1:A:149:LYS:HE3	3:A:318:HOH:O	2.08	0.53
1:A:33:LEU:HD12	1:A:36:LEU:HD12	1.91	0.52
1:A:59:LYS:NZ	3:A:454:HOH:O	2.43	0.52
1:A:106:SER:O	1:A:110:GLU:HG2	2.09	0.51
1:A:64:LYS:HE3	1:A:66:PHE:CE1	2.46	0.51
1:A:40:TYR:OH	1:A:277:LYS:HB3	2.10	0.51
1:A:122:LEU:HD22	1:A:134:ALA:HA	1.92	0.50
1:A:112:TYR:CE2	1:A:117:ILE:HG13	2.46	0.50
1:A:96:HIS:HA	1:A:116:ASP:OD1	2.12	0.50
1:A:222:LYS:HE3	1:A:233:ASP:OD1	2.11	0.49
1:A:124:GLU:OE2	3:A:326:HOH:O	2.19	0.49
1:A:178:LYS:HB2	1:A:178:LYS:HZ3	1.77	0.49
1:A:62:SER:O	1:A:183:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HE3	1:A:66:PHE:CZ	2.49	0.48
1:A:220:LEU:CD1	1:A:235:SER:HB2	2.44	0.48
1:A:104:ALA:HB3	1:A:167:ILE:HD13	1.94	0.48
1:A:251:TYR:CZ	1:A:258:PRO:HB3	2.49	0.47
1:A:242:ALA:HB2	1:A:272:ASP:O	2.14	0.47
1:A:153:LYS:HG3	1:A:154:GLU:H	1.79	0.47
1:A:127:MET:HE3	1:A:127:MET:HB3	1.77	0.46
1:A:126:SER:O	1:A:130:SER:HA	2.14	0.46
1:A:220:LEU:HD12	1:A:235:SER:HB3	1.98	0.46
1:A:31:LYS:N	1:A:31:LYS:CD	2.79	0.46
1:A:233:ASP:OD2	1:A:246:ASP:OD1	2.34	0.45
1:A:274:PRO:O	3:A:372:HOH:O	2.21	0.45
1:A:84:VAL:HA	1:A:87:PRO:HD2	1.80	0.45
1:A:44:ILE:O	1:A:61:ASN:HB2	2.17	0.44
1:A:222:LYS:HG3	3:A:309:HOH:O	2.15	0.44
1:A:196:ASN:HB2	3:A:431:HOH:O	2.18	0.44
1:A:224:GLY:HA3	1:A:280:SER:O	2.17	0.44
1:A:149:LYS:HD2	1:A:162:PRO:HD2	2.01	0.43
1:A:194:ILE:O	1:A:204:LYS:HD2	2.19	0.43
1:A:33:LEU:HD21	1:A:46:VAL:HG21	2.00	0.43
1:A:222:LYS:HG2	1:A:231:VAL:HB	2.01	0.42
1:A:242:ALA:HB2	1:A:272:ASP:C	2.44	0.42
1:A:93:LYS:CD	3:A:411:HOH:O	2.67	0.41
1:A:98:ASN:HB2	3:A:428:HOH:O	2.20	0.41
1:A:251:TYR:CE2	1:A:258:PRO:HB3	2.56	0.41
1:A:44:ILE:HG22	1:A:46:VAL:HG23	2.02	0.41
1:A:150:GLN:O	1:A:153:LYS:HG2	2.20	0.41
1:A:170:ASN:HB2	1:A:239:ILE:HD12	2.02	0.41
1:A:43:HIS:HB3	1:A:64:LYS:NZ	2.37	0.40
1:A:220:LEU:HD12	1:A:235:SER:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	218/227 (96%)	195 (89%)	23 (11%)	6 8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	35	ASP
1	A	75	ILE
1	A	111	LYS
1	A	117	ILE
1	A	145	ILE
1	A	146	LYS
1	A	153	LYS
1	A	158	LYS
1	A	168	GLU
1	A	194	ILE
1	A	201	LYS
1	A	202	GLU
1	A	204	LYS
1	A	216	SER
1	A	229	TYR
1	A	233	ASP
1	A	237	GLN
1	A	277	LYS
1	A	280	SER
1	A	284	LYS
1	A	285	SER
1	A	289	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	150	GLN
1	A	196	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](#)

1 ligand is 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	FOS	A	291	1	12,15,16	1.25	2 (16%)	14,18,21	2.71	6 (42%)

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	FOS	A	291	1	-	3/8/10/11	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	291	FOS	C3-C2	2.43	1.43	1.38
2	A	291	FOS	C2-C1	2.15	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	291	FOS	O-C'-N	7.09	122.31	110.62
2	A	291	FOS	O'-C'-N	-3.84	119.14	124.93
2	A	291	FOS	O-C'-O'	-3.00	118.51	124.26
2	A	291	FOS	C6-C1-C2	2.79	122.39	118.23
2	A	291	FOS	C5-C4-C3	2.58	123.40	119.87
2	A	291	FOS	C3-C2-C1	-2.40	117.23	120.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	291	FOS	P-CM-N-C'
2	A	291	FOS	O'-C'-O-C
2	A	291	FOS	N-C'-O-C

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	291	FOS	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.