



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:36 PM GMT

PDB ID : 1BLS
Title : CRYSTALLOGRAPHIC STRUCTURE OF A PHOSPHONATE DERIVATIVE OF THE ENTEROBACTER CLOACAE P99 CEPHALOSPORINASE: MECHANISTIC INTERPRETATION OF A BETA-LACTAMASE TRANSITION STATE ANALOG
Authors : Knox, J.R.; Moews, P.C.; Lobkovsky, E.
Deposited on : 1993-12-17
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

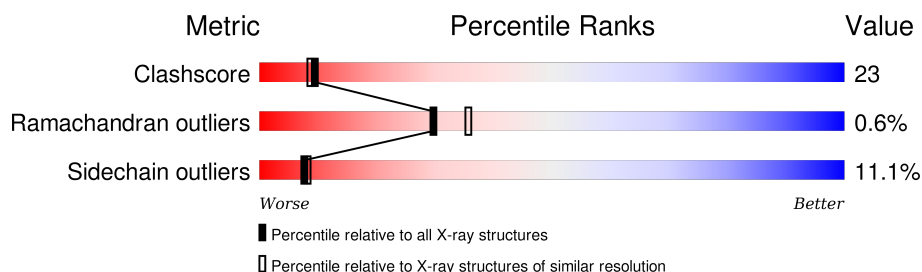
1 Overall quality at a glance

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	 64% 29% 6% ..
1	B	361	 65% 29% 5% ..

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	IPP	A	362[B]	-	-	X	-
2	IPP	B	362[B]	-	-	X	-

2 Entry composition [i](#)

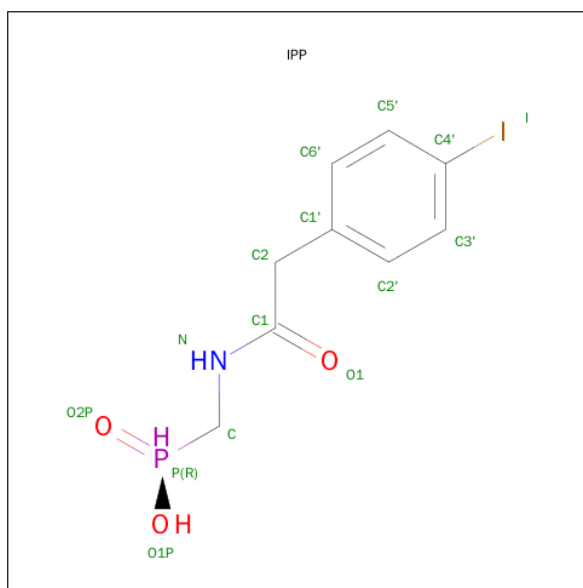
There are 3 unique types of molecules in this entry. The entry contains 6341 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	359	Total	C	N	O	S	0	0	0
			2751	1768	465	506	12			
1	B	359	Total	C	N	O	S	0	0	0
			2751	1768	465	506	12			

- Molecule 2 is (P-IODOPHENYLACETYLAMINO)METHYLPHOSPHINIC ACID (three-letter code: IPP) (formula: C₉H₁₁INO₃P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	P	0	1
			25	17	2	1	4	1		
2	B	1	Total	C	I	N	O	P	0	1
			25	17	2	1	4	1		

- Molecule 3 is water.

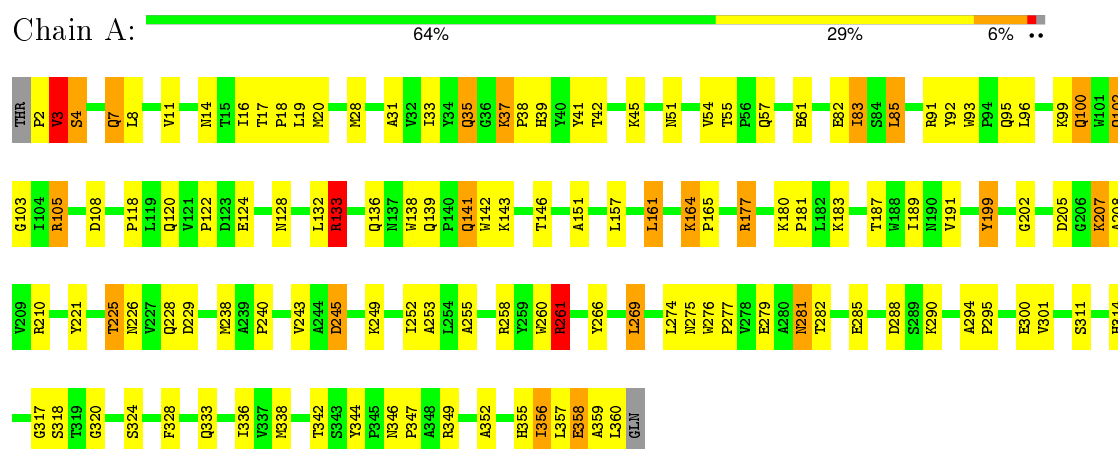
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	397	Total 397	O 397	0	0
3	B	392	Total 392	O 392	0	0

3 Residue-property plots

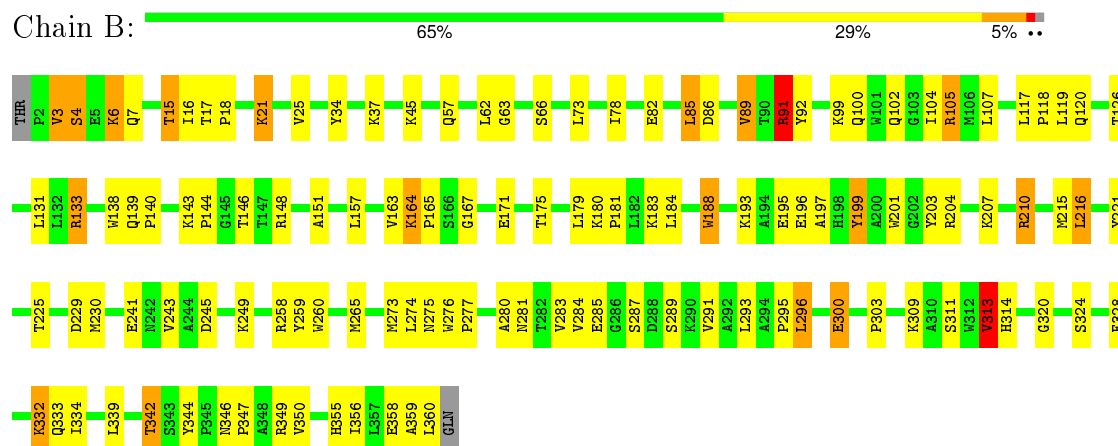
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: BETA-LACTAMASE



• Molecule 1: BETA-LACTAMASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.50Å 83.47Å 95.46Å 90.00° 90.01° 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}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6341	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.70	0/2827	1.11	8/3863 (0.2%)
1	B	0.71	0/2827	1.14	7/3863 (0.2%)
All	All	0.71	0/5654	1.12	15/7726 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ARG	CD-NE-CZ	16.13	146.19	123.60
1	B	210	ARG	NE-CZ-NH1	10.91	125.76	120.30
1	B	91	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	177	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	133	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	105	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	177	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	91	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	274	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	261	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	313	VAL	CB-CA-C	5.46	121.77	111.40
1	A	342	THR	N-CA-CB	5.18	120.15	110.30
1	B	210	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	177	ARG	CD-NE-CZ	5.05	130.68	123.60
1	A	133	ARG	CD-NE-CZ	5.05	130.66	123.60

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	2751	0	2737	128	5
1	B	2751	0	2737	121	3
2	A	25	0	13	7	0
2	B	25	0	14	7	0
3	A	397	0	0	36	5
3	B	392	0	0	37	4
All	All	6341	0	5501	250	9

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 (250) 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:143:LYS:HG2	3:A:410:HOH:O	1.17	1.27
1:B:259:TYR:HB2	3:B:731:HOH:O	1.45	1.15
1:A:279:GLU:HB2	3:A:503:HOH:O	1.47	1.14
1:A:128:ASN:HB3	3:A:506:HOH:O	1.55	1.06
1:A:355:HIS:O	1:A:358:GLU:HG3	1.56	1.04
1:B:175:THR:HG22	1:B:180:LYS:HE2	1.38	1.03
1:B:15:THR:HG21	1:B:356:ILE:HD11	1.41	1.03
1:A:258:ARG:HH12	1:A:275:ASN:ND2	1.56	1.01
1:B:99:LYS:HE3	3:B:621:HOH:O	1.62	0.98
1:A:281:ASN:HB2	3:A:593:HOH:O	1.65	0.97
1:A:238:MET:HE3	1:A:328:PHE:HB2	1.47	0.94
1:A:42:THR:HG21	1:A:54:VAL:O	1.68	0.94
1:A:258:ARG:HH12	1:A:275:ASN:HD21	0.94	0.91
1:A:164:LYS:HD3	1:A:165:PRO:HD3	1.54	0.89
1:B:258:ARG:HH12	1:B:275:ASN:HD21	1.14	0.89
1:B:295:PRO:O	1:B:296:LEU:HD22	1.73	0.88
1:B:175:THR:HG22	1:B:180:LYS:CE	2.05	0.86
1:B:133:ARG:NH1	3:B:646:HOH:O	2.09	0.85
1:A:42:THR:HG23	1:A:54:VAL:HG12	1.59	0.85
1:B:283:VAL:HG12	1:B:350:VAL:HG11	1.58	0.85
1:B:280:ALA:O	1:B:284:VAL:HG22	1.77	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LYS:HG2	3:B:595:HOH:O	1.76	0.84
1:A:360:LEU:HB3	3:A:747:HOH:O	1.78	0.83
1:B:295:PRO:O	1:B:296:LEU:CD2	2.27	0.82
1:B:105:ARG:NH2	1:B:107:LEU:HD23	1.96	0.81
1:A:122:PRO:HA	3:A:460:HOH:O	1.79	0.81
1:B:15:THR:CG2	1:B:356:ILE:HD11	2.11	0.80
1:A:281:ASN:HB3	3:A:640:HOH:O	1.82	0.79
1:A:258:ARG:NH1	1:A:275:ASN:HD21	1.77	0.79
1:A:360:LEU:C	3:A:555:HOH:O	2.21	0.79
1:B:15:THR:HG21	1:B:356:ILE:CD1	2.13	0.78
1:A:37:LYS:HZ2	1:A:38:PRO:HD2	1.50	0.77
1:B:197:ALA:HB3	3:B:752:HOH:O	1.84	0.76
1:B:243:VAL:O	1:B:249:LYS:HE3	1.87	0.75
1:B:260:TRP:CD1	3:B:731:HOH:O	2.40	0.74
1:B:105:ARG:HH21	1:B:107:LEU:HD23	1.51	0.74
1:A:37:LYS:HA	1:A:37:LYS:NZ	2.02	0.74
1:A:42:THR:CG2	1:A:54:VAL:O	2.36	0.74
1:A:37:LYS:HA	1:A:37:LYS:HZ3	1.52	0.73
1:B:295:PRO:C	1:B:296:LEU:HD23	2.10	0.73
1:A:243:VAL:O	1:A:249:LYS:HE3	1.88	0.73
1:B:188:TRP:CZ2	1:B:195:GLU:HG3	2.23	0.73
1:A:288:ASP:OD2	1:A:290:LYS:HG2	1.89	0.72
1:A:82:GLU:O	1:A:83:ILE:HD12	1.89	0.72
1:A:358:GLU:C	1:A:360:LEU:H	1.92	0.71
1:A:143:LYS:HG3	1:A:146:THR:HG21	1.71	0.71
1:A:221:TYR:CD1	2:A:362[B]:IPP:H6'	2.25	0.71
1:B:287:SER:OG	1:B:350:VAL:HG21	1.89	0.70
1:B:273:MET:HG3	1:B:313:VAL:HB	1.75	0.69
1:B:355:HIS:NE2	3:B:624:HOH:O	2.26	0.69
1:B:358:GLU:CG	3:B:733:HOH:O	2.40	0.69
1:B:258:ARG:HH12	1:B:275:ASN:ND2	1.90	0.68
1:A:141:GLN:NE2	3:A:470:HOH:O	2.26	0.67
1:A:357:LEU:O	1:A:360:LEU:HD23	1.95	0.66
1:B:199:TYR:CZ	1:B:210:ARG:HD3	2.29	0.66
1:B:241:GLU:HG3	3:B:644:HOH:O	1.93	0.66
1:A:336:ILE:HD12	1:A:356:ILE:HG12	1.76	0.65
1:B:358:GLU:HB3	3:B:733:HOH:O	1.96	0.65
1:B:86:ASP:HB3	3:B:661:HOH:O	1.97	0.65
1:A:61:GLU:O	3:A:589:HOH:O	2.14	0.65
1:B:295:PRO:C	1:B:296:LEU:CD2	2.66	0.64
1:B:283:VAL:HG12	1:B:350:VAL:CG1	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:VAL:HG22	3:A:457:HOH:O	1.98	0.64
1:A:7:GLN:O	1:A:11:VAL:HG23	1.98	0.64
1:A:83:ILE:CD1	1:A:165:PRO:HG2	2.27	0.64
1:B:118:PRO:O	1:B:151:ALA:HB1	1.97	0.64
1:B:120:GLN:OE1	2:B:362[B]:IPP:C5'	2.45	0.63
1:A:164:LYS:HD3	1:A:165:PRO:CD	2.28	0.63
1:A:221:TYR:CE1	2:A:362[B]:IPP:H6'	2.33	0.63
1:A:255:ALA:HA	1:A:269:LEU:HB2	1.81	0.62
1:B:15:THR:HG22	1:B:16:ILE:HG12	1.82	0.62
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.65	0.62
1:B:225:THR:HG21	1:B:230:MET:HE2	1.82	0.62
1:A:28:MET:HE3	1:A:338:MET:HB3	1.80	0.62
1:B:221:TYR:CZ	2:B:362[B]:IPP:C3'	2.83	0.61
1:A:333:GLN:HG2	3:A:714:HOH:O	1.99	0.61
1:B:265:MET:CE	3:B:412:HOH:O	2.48	0.61
1:A:324:SER:OG	3:A:589:HOH:O	2.16	0.60
1:A:261:ARG:NH1	3:A:566:HOH:O	2.34	0.60
1:B:143:LYS:HG3	1:B:146:THR:CG2	2.31	0.60
1:B:15:THR:O	1:B:18:PRO:HD2	2.00	0.59
1:A:290:LYS:NZ	3:A:727:HOH:O	2.36	0.59
1:B:82:GLU:OE1	3:B:379:HOH:O	2.17	0.59
1:B:105:ARG:HD3	3:B:536:HOH:O	2.02	0.59
1:A:14:ASN:OD1	3:A:623:HOH:O	2.17	0.59
1:B:355:HIS:CD2	3:B:624:HOH:O	2.56	0.58
1:B:241:GLU:OE2	3:B:644:HOH:O	2.17	0.58
1:A:118:PRO:O	1:A:151:ALA:HB1	2.03	0.58
1:A:346:ASN:HB2	1:A:347:PRO:HD3	1.85	0.58
1:B:126:THR:OG1	3:B:732:HOH:O	2.16	0.58
1:A:42:THR:HG21	1:A:54:VAL:C	2.24	0.58
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.40	0.57
1:A:183:LYS:HE2	3:A:704:HOH:O	2.04	0.57
1:B:175:THR:HA	1:B:179:LEU:HB2	1.87	0.57
1:B:221:TYR:CD1	2:B:362[B]:IPP:H2'	2.40	0.57
1:B:143:LYS:HG3	1:B:146:THR:HG21	1.87	0.57
1:B:15:THR:HG21	1:B:356:ILE:CG1	2.35	0.56
1:A:100:GLN:OE1	1:A:138:TRP:O	2.24	0.56
1:B:17:THR:O	1:B:21:LYS:HD2	2.06	0.56
1:A:102:GLN:HG3	1:A:103:GLY:N	2.21	0.56
1:A:37:LYS:NZ	1:A:38:PRO:HD2	2.19	0.55
1:A:253:ALA:HB2	3:A:657:HOH:O	2.06	0.55
1:B:358:GLU:CD	3:B:733:HOH:O	2.44	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ALA:O	1:A:356:ILE:HG23	2.07	0.55
1:B:196:GLU:HG3	3:B:581:HOH:O	2.07	0.55
1:B:89:VAL:HG12	1:B:104:ILE:O	2.06	0.55
1:A:42:THR:HG23	1:A:54:VAL:CG1	2.34	0.54
1:A:187:THR:OG1	1:A:225:THR:HG23	2.07	0.54
1:A:2:PRO:HG3	1:A:35:GLN:HE22	1.71	0.54
1:A:282:THR:HG23	3:A:671:HOH:O	2.08	0.54
1:A:17:THR:HB	1:A:18:PRO:HD3	1.90	0.54
1:B:133:ARG:CZ	3:B:399:HOH:O	2.54	0.54
1:A:55:THR:C	3:A:547:HOH:O	2.46	0.54
1:A:143:LYS:CG	3:A:410:HOH:O	2.03	0.53
1:B:221:TYR:CZ	2:B:362[B]:IPP:H3'	2.43	0.53
1:A:143:LYS:HG3	1:A:146:THR:CG2	2.37	0.53
1:A:258:ARG:NH1	1:A:275:ASN:ND2	2.41	0.53
1:A:99:LYS:O	1:A:99:LYS:HG2	2.08	0.53
1:A:199:TYR:O	1:A:210:ARG:NH2	2.42	0.53
1:A:183:LYS:HG2	3:A:722:HOH:O	2.08	0.53
1:A:35:GLN:NE2	3:A:598:HOH:O	2.40	0.53
1:B:221:TYR:CE1	2:B:362[B]:IPP:H2'	2.43	0.53
1:A:261:ARG:HG3	1:A:266:TYR:CE2	2.44	0.53
1:B:164:LYS:CB	1:B:165:PRO:HD3	2.38	0.53
1:B:171:GLU:OE2	3:B:410:HOH:O	2.18	0.52
1:A:225:THR:HG22	1:A:229:ASP:HB2	1.91	0.52
1:A:180:LYS:HB2	1:A:181:PRO:HD3	1.91	0.52
1:B:259:TYR:CB	3:B:731:HOH:O	2.26	0.52
1:A:2:PRO:O	1:A:3:VAL:HG13	2.09	0.52
1:B:4:SER:CB	1:B:7:GLN:HE21	2.22	0.52
1:A:164:LYS:CB	1:A:165:PRO:HD3	2.40	0.52
1:B:281:ASN:O	1:B:285:GLU:HB2	2.10	0.51
1:A:3:VAL:HG23	1:A:4:SER:H	1.75	0.51
1:B:260:TRP:N	3:B:731:HOH:O	2.44	0.51
1:A:133:ARG:CG	1:A:133:ARG:HH11	2.23	0.51
1:A:358:GLU:C	1:A:360:LEU:N	2.64	0.51
1:B:346:ASN:N	1:B:347:PRO:CD	2.74	0.51
1:A:83:ILE:HD11	1:A:92:TYR:CE1	2.46	0.50
1:B:184:LEU:HD23	3:B:629:HOH:O	2.10	0.50
1:B:15:THR:CG2	1:B:16:ILE:HG12	2.42	0.50
1:A:281:ASN:O	1:A:285:GLU:HB3	2.11	0.50
1:B:295:PRO:O	1:B:296:LEU:HD23	2.07	0.50
1:B:183:LYS:HA	3:B:475:HOH:O	2.12	0.50
1:A:189:ILE:HG13	3:A:683:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:CD	1:A:165:PRO:HD3	2.36	0.50
1:B:6:LYS:HB2	1:B:6:LYS:HZ3	1.77	0.50
1:A:105:ARG:HD3	1:A:108:ASP:OD2	2.12	0.50
1:A:92:TYR:HD1	1:A:164:LYS:CD	2.24	0.50
1:B:332:LYS:HB3	1:B:334:ILE:HG12	1.93	0.50
1:A:120:GLN:HE22	2:A:362[B]:IPP:C2'	2.24	0.49
1:B:167:GLY:HA2	3:B:681:HOH:O	2.11	0.49
1:A:120:GLN:NE2	2:A:362[B]:IPP:C3'	2.74	0.49
1:A:180:LYS:CB	1:A:181:PRO:HD3	2.42	0.49
1:A:360:LEU:O	3:A:597:HOH:O	2.20	0.49
2:A:362[B]:IPP:I	3:A:563:HOH:O	2.90	0.49
1:B:260:TRP:HD1	3:B:731:HOH:O	1.86	0.49
1:A:100:GLN:NE2	1:A:136:GLN:O	2.46	0.49
1:B:143:LYS:HB2	1:B:144:PRO:HD2	1.95	0.49
1:B:204:ARG:HG2	1:B:320:GLY:O	2.12	0.49
1:A:143:LYS:CE	3:A:410:HOH:O	2.60	0.49
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.48	0.48
1:B:17:THR:HB	1:B:18:PRO:HD3	1.95	0.48
1:A:164:LYS:HB3	1:A:165:PRO:HD3	1.96	0.48
1:A:346:ASN:CB	1:A:347:PRO:HD3	2.43	0.48
1:A:143:LYS:HE2	3:A:410:HOH:O	2.12	0.48
1:B:167:GLY:CA	3:B:681:HOH:O	2.61	0.48
1:B:215:MET:O	1:B:216:LEU:HB2	2.13	0.48
1:B:133:ARG:HD2	3:B:646:HOH:O	2.13	0.48
1:B:313:VAL:HG22	1:B:328:PHE:CZ	2.49	0.48
1:B:300:GLU:HG2	1:B:300:GLU:O	2.11	0.47
1:B:175:THR:CG2	1:B:180:LYS:HE2	2.27	0.47
1:B:289:SER:O	1:B:293:LEU:HB2	2.14	0.47
1:A:344:TYR:CE2	1:A:349:ARG:HG2	2.48	0.47
1:A:240:PRO:O	1:A:249:LYS:HE2	2.14	0.47
1:B:25:VAL:HG22	1:B:342:THR:HG22	1.96	0.47
1:B:62:LEU:HD11	1:B:230:MET:HE3	1.96	0.47
1:B:207:LYS:HB3	1:B:207:LYS:HE3	1.65	0.47
1:B:258:ARG:NH2	1:B:311:SER:OG	2.48	0.47
1:A:356:ILE:HG13	1:A:357:LEU:N	2.30	0.47
1:B:120:GLN:CD	2:B:362[B]:IPP:C5'	2.83	0.47
1:A:138:TRP:NE1	3:A:540:HOH:O	2.33	0.47
1:B:25:VAL:HG22	1:B:342:THR:CG2	2.45	0.47
1:B:324:SER:HB3	1:B:339:LEU:HD23	1.96	0.46
1:A:260:TRP:CZ3	1:A:300:GLU:HG3	2.50	0.46
1:A:226:ASN:OD1	1:A:228:GLN:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TRP:CZ2	1:B:140:PRO:HB3	2.51	0.46
1:A:205:ASP:O	1:A:207:LYS:HD2	2.15	0.46
1:B:139:GLN:NE2	3:B:529:HOH:O	2.48	0.46
1:B:15:THR:CG2	1:B:16:ILE:N	2.78	0.45
1:B:120:GLN:CD	2:B:362[B]:IPP:H5'	2.36	0.45
1:B:358:GLU:OE1	3:B:733:HOH:O	2.19	0.45
1:B:265:MET:CE	3:B:424:HOH:O	2.64	0.45
1:A:57:GLN:NE2	1:A:228:GLN:OE1	2.49	0.45
1:A:31:ALA:HA	1:A:39:HIS:O	2.17	0.45
1:B:148:ARG:O	1:B:295:PRO:HA	2.16	0.45
1:A:164:LYS:CE	1:A:165:PRO:HG3	2.47	0.45
1:A:4:SER:O	1:A:7:GLN:N	2.50	0.45
1:B:265:MET:HE1	3:B:424:HOH:O	2.16	0.45
1:B:138:TRP:CH2	1:B:140:PRO:HB3	2.52	0.45
1:B:175:THR:HG22	1:B:180:LYS:NZ	2.32	0.45
1:B:146:THR:HB	3:B:495:HOH:O	2.17	0.45
1:A:358:GLU:HA	3:A:699:HOH:O	2.16	0.45
1:A:2:PRO:HG3	1:A:35:GLN:NE2	2.32	0.45
1:B:102:GLN:NE2	3:B:632:HOH:O	2.50	0.44
1:A:157:LEU:HG	1:A:161:LEU:HD22	1.99	0.44
1:A:320:GLY:N	3:A:459:HOH:O	2.47	0.44
1:A:346:ASN:N	1:A:347:PRO:CD	2.80	0.44
1:A:221:TYR:CG	2:A:362[B]:IPP:H22	2.53	0.44
1:B:143:LYS:CG	1:B:146:THR:HG21	2.46	0.43
1:B:91:ARG:HD3	1:B:92:TYR:CZ	2.52	0.43
1:A:294:ALA:HA	1:A:295:PRO:HD3	1.86	0.43
1:B:359:ALA:O	1:B:360:LEU:HD23	2.18	0.43
1:A:93:TRP:CE3	1:A:96:LEU:HD22	2.53	0.43
1:A:17:THR:N	1:A:18:PRO:CD	2.82	0.43
1:A:93:TRP:CD1	1:A:95:GLN:NE2	2.87	0.43
1:B:3:VAL:N	1:B:34:TYR:OH	2.51	0.43
1:A:199:TYR:OH	3:A:465:HOH:O	2.21	0.43
1:B:281:ASN:HA	1:B:284:VAL:CG2	2.49	0.43
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.53	0.43
1:B:3:VAL:HA	1:B:34:TYR:HE2	1.84	0.42
1:A:221:TYR:CB	2:A:362[B]:IPP:H22	2.49	0.42
1:B:201:TRP:CZ3	1:B:210:ARG:HG3	2.54	0.42
1:A:240:PRO:HB3	1:A:252:ILE:HG21	2.01	0.42
1:A:45:LYS:NZ	3:A:490:HOH:O	2.52	0.42
1:B:180:LYS:HB2	1:B:181:PRO:HD3	2.01	0.42
1:B:17:THR:N	1:B:18:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:CG2	1:A:54:VAL:C	2.86	0.42
1:B:203:TYR:HA	1:B:207:LYS:O	2.20	0.42
1:A:164:LYS:NZ	1:A:165:PRO:HG3	2.34	0.42
1:A:202:GLY:O	1:A:208:ALA:HA	2.20	0.42
1:A:245:ASP:CG	3:A:438:HOH:O	2.57	0.42
1:A:128:ASN:HB2	3:A:697:HOH:O	2.20	0.42
1:B:346:ASN:HB2	1:B:347:PRO:HD3	2.02	0.42
1:B:78:ILE:HD13	1:B:85:LEU:HD22	2.01	0.41
1:A:85:LEU:HA	1:A:85:LEU:HD12	1.92	0.41
1:B:63:GLY:O	1:B:66:SER:HB2	2.19	0.41
1:A:359:ALA:O	1:A:360:LEU:C	2.58	0.41
1:A:8:LEU:HD23	1:A:41:TYR:OH	2.20	0.41
1:B:143:LYS:HG3	1:B:146:THR:HG23	2.03	0.41
1:B:313:VAL:HG22	1:B:328:PHE:CE2	2.56	0.41
1:A:141:GLN:HG2	1:A:142:TRP:CZ2	2.56	0.41
1:A:16:ILE:O	1:A:20:MET:HG3	2.21	0.41
1:A:55:THR:O	3:A:547:HOH:O	2.22	0.40
1:B:139:GLN:CD	3:B:529:HOH:O	2.59	0.40
1:B:100:GLN:O	1:B:104:ILE:CD1	2.70	0.40
1:A:180:LYS:N	1:A:181:PRO:CD	2.84	0.40
1:B:229:ASP:OD1	3:B:446:HOH:O	2.22	0.40
1:B:4:SER:CB	1:B:7:GLN:NE2	2.84	0.40

All (9) 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)
3:B:542:HOH:O	3:B:577:HOH:O[1_455]	1.73	0.47
3:A:507:HOH:O	3:B:436:HOH:O[2_655]	1.89	0.31
1:A:277:PRO:CG	3:A:678:HOH:O[1_655]	1.90	0.30
1:A:164:LYS:NZ	1:B:303:PRO:CG[2_555]	1.96	0.24
1:A:277:PRO:CD	3:A:678:HOH:O[1_655]	2.03	0.17
1:A:143:LYS:NZ	1:B:143:LYS:CD[1_665]	2.06	0.14
3:A:399:HOH:O	3:B:654:HOH:O[1_665]	2.08	0.12
3:A:472:HOH:O	3:B:471:HOH:O[1_665]	2.14	0.06
1:A:164:LYS:NZ	1:B:303:PRO:CB[2_555]	2.17	0.03

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	357/361 (99%)	341 (96%)	14 (4%)	2 (1%)	30	36
1	B	357/361 (99%)	343 (96%)	12 (3%)	2 (1%)	30	36
All	All	714/722 (99%)	684 (96%)	26 (4%)	4 (1%)	30	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	4	SER
1	B	4	SER
1	B	3	VAL

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	285/287 (99%)	252 (88%)	33 (12%)	7	7
1	B	285/287 (99%)	255 (90%)	30 (10%)	8	9
All	All	570/574 (99%)	507 (89%)	63 (11%)	8	8

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	19	LEU
1	A	33	ILE
1	A	35	GLN
1	A	37	LYS
1	A	51	ASN
1	A	83	ILE
1	A	85	LEU
1	A	100	GLN
1	A	102	GLN
1	A	105	ARG
1	A	124	GLU
1	A	132	LEU
1	A	133	ARG
1	A	139	GLN
1	A	141	GLN
1	A	161	LEU
1	A	164	LYS
1	A	177	ARG
1	A	191	VAL
1	A	199	TYR
1	A	207	LYS
1	A	225	THR
1	A	245	ASP
1	A	261	ARG
1	A	269	LEU
1	A	274	LEU
1	A	281	ASN
1	A	311	SER
1	A	314	HIS
1	A	356	ILE
1	A	358	GLU
1	B	6	LYS
1	B	15	THR
1	B	21	LYS
1	B	37	LYS
1	B	45	LYS
1	B	57	GLN
1	B	73	LEU
1	B	85	LEU
1	B	89	VAL
1	B	91	ARG
1	B	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	119	LEU
1	B	131	LEU
1	B	133	ARG
1	B	157	LEU
1	B	163	VAL
1	B	164	LYS
1	B	188	TRP
1	B	193	LYS
1	B	199	TYR
1	B	216	LEU
1	B	245	ASP
1	B	291	VAL
1	B	296	LEU
1	B	300	GLU
1	B	313	VAL
1	B	314	HIS
1	B	332	LYS
1	B	333	GLN
1	B	342	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	GLN
1	A	57	GLN
1	A	102	GLN
1	A	137	ASN
1	A	186	HIS
1	A	198	HIS
1	A	242	ASN
1	A	250	GLN
1	A	275	ASN
1	A	355	HIS
1	B	7	GLN
1	B	35	GLN
1	B	137	ASN
1	B	275	ASN
1	B	346	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	IPP	A	362[A]	-	11,15,15	1.86	1 (9%)	14,19,19	5.66	5 (35%)
2	IPP	A	362[B]	-	11,15,15	1.39	1 (9%)	14,19,19	5.20	5 (35%)
2	IPP	B	362[A]	-	11,15,15	2.22	2 (18%)	14,19,19	5.38	4 (28%)
2	IPP	B	362[B]	-	11,15,15	2.11	1 (9%)	14,19,19	4.16	5 (35%)

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	IPP	A	362[A]	-	-	0/7/9/9	0/1/1/1
2	IPP	A	362[B]	-	-	0/7/9/9	0/1/1/1
2	IPP	B	362[A]	-	-	0/7/9/9	0/1/1/1
2	IPP	B	362[B]	-	-	0/7/9/9	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	362[A]	IPP	C2-C1	-6.60	1.35	1.51
2	B	362[B]	IPP	C2-C1	-6.48	1.35	1.51
2	A	362[A]	IPP	C2-C1	-5.65	1.37	1.51
2	A	362[B]	IPP	C2-C1	-3.96	1.42	1.51
2	B	362[A]	IPP	O1-C1	2.45	1.28	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	362[A]	IPP	O1-C1-C2	-10.06	93.78	121.88
2	B	362[A]	IPP	O1-C1-C2	-9.92	94.16	121.88
2	A	362[B]	IPP	O1-C1-C2	-8.78	97.34	121.88
2	B	362[B]	IPP	O1-C1-C2	-6.82	102.82	121.88
2	B	362[B]	IPP	C3'-C4'-I	-2.49	115.76	119.67
2	A	362[B]	IPP	C3'-C4'-I	-2.47	115.78	119.67
2	A	362[A]	IPP	C3'-C4'-I	-2.46	115.80	119.67
2	B	362[A]	IPP	C3'-C4'-I	-2.44	115.83	119.67
2	B	362[B]	IPP	C5'-C4'-I	2.01	122.83	119.67
2	A	362[A]	IPP	C5'-C4'-I	2.04	122.88	119.67
2	A	362[B]	IPP	C5'-C4'-I	2.08	122.94	119.67
2	B	362[B]	IPP	C1'-C2-C1	2.81	121.99	112.84
2	A	362[A]	IPP	C1'-C2-C1	3.85	125.38	112.84
2	A	362[B]	IPP	C1'-C2-C1	4.54	127.66	112.84
2	B	362[A]	IPP	C1'-C2-C1	4.85	128.65	112.84
2	B	362[B]	IPP	C2-C1-N	13.17	134.61	116.11
2	A	362[B]	IPP	C2-C1-N	16.32	139.03	116.11
2	B	362[A]	IPP	C2-C1-N	16.39	139.13	116.11
2	A	362[A]	IPP	C2-C1-N	17.83	141.15	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	362[B]	IPP	7	0
2	B	362[B]	IPP	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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