



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 1CP9 / pdb_00001cp9
Title : CRYSTAL STRUCTURE OF PENICILLIN G ACYLASE FROM THE BRO1
MUTANT STRAIN OF PROVIDENCIA RETTGERI
Authors : McDonough, M.A.; Klei, H.E.; Kelly, J.A.
Deposited on : 1999-06-12
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

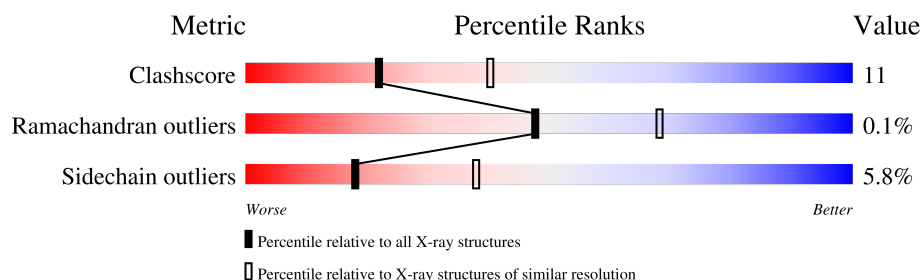
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	205	
2	B	553	

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
3	SO4	B	556	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6814 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 Penicillin G amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1609	1024	261	317	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	LEU	MET	engineered mutation	UNP Q7WZI9

- Molecule 2 is a protein called Penicillin G amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	553	Total	C	N	O	S	0	0	0
			4408	2811	753	838	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	201	Total O 201 201	0	0
5	B	575	Total O 575 575	0	0

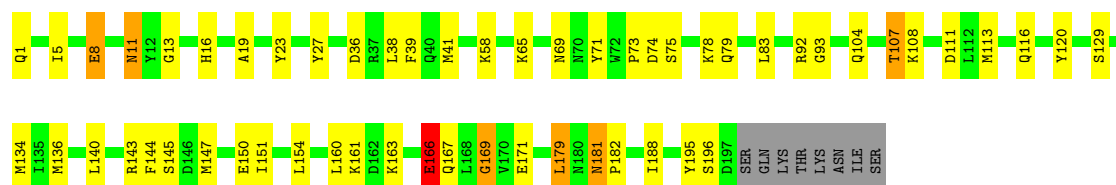
3 Residue-property plots

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. 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.

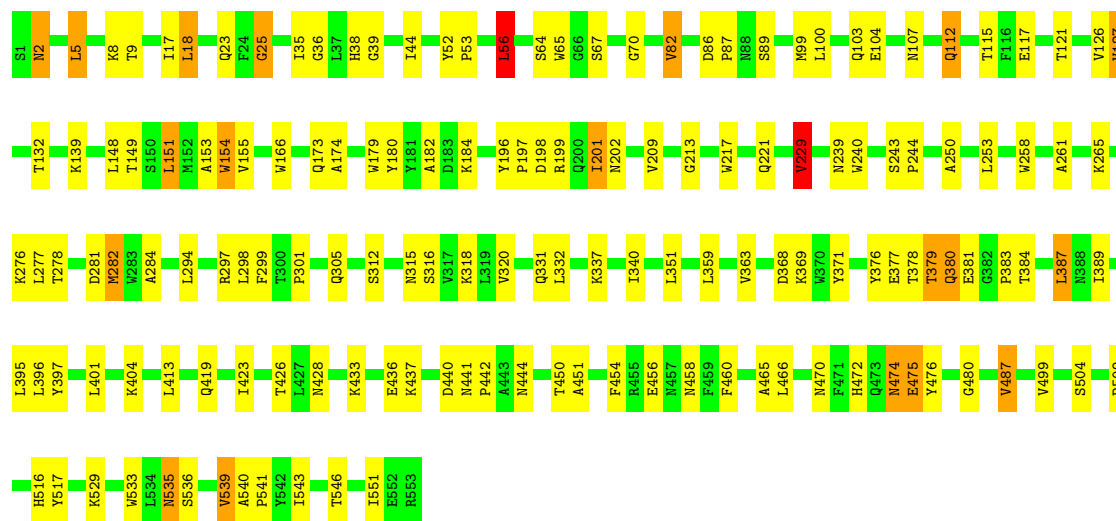
• Molecule 1: Penicillin G amidase

Chain A: 



• Molecule 2: Penicillin G amidase

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	140.65Å 140.65Å 200.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	86.7 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.154 , 0.165	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6814	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: CA, PCA, SO4

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	0.87	0/1642	1.24	12/2229 (0.5%)
2	B	0.89	3/4541 (0.1%)	1.17	27/6191 (0.4%)
All	All	0.89	3/6183 (0.0%)	1.19	39/8420 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	282	MET	SD-CE	-9.61	1.55	1.79
2	B	499	VAL	CA-CB	6.53	1.60	1.53
2	B	487	VAL	CA-CB	5.22	1.61	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASP	N-CA-C	10.14	122.41	111.36
2	B	153	ALA	N-CA-C	-9.63	100.65	111.82
2	B	389	ILE	N-CA-C	-7.85	98.52	108.89
2	B	299	PHE	N-CA-C	7.81	123.12	112.90
2	B	25	GLY	N-CA-C	-7.63	101.49	112.17
2	B	380	GLN	N-CA-C	-7.13	103.58	111.36
2	B	536	SER	N-CA-C	6.59	119.31	111.33
2	B	535	ASN	N-CA-C	6.55	120.74	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	GLY	N-CA-C	6.49	120.52	113.58
1	A	83	LEU	CA-C-N	-6.44	113.66	120.03
1	A	83	LEU	C-N-CA	-6.44	113.66	120.03
1	A	179	LEU	N-CA-C	-6.40	103.60	111.40
1	A	58	LYS	N-CA-C	6.16	118.78	111.33
2	B	70	GLY	N-CA-C	5.92	122.74	113.86
2	B	174	ALA	N-CA-C	5.92	120.66	113.38
2	B	294	LEU	N-CA-C	5.91	118.68	111.82
2	B	67	SER	N-CA-C	5.83	117.00	108.14
1	A	38	LEU	N-CA-C	5.76	118.03	111.11
2	B	100	LEU	N-CA-C	-5.76	102.38	110.50
1	A	169	GLY	N-CA-C	-5.71	105.88	112.73
2	B	198	ASP	N-CA-C	-5.67	97.21	107.75
1	A	181	ASN	CA-C-N	5.66	125.33	119.56
1	A	181	ASN	C-N-CA	5.66	125.33	119.56
2	B	56	LEU	N-CA-C	5.58	117.44	111.36
2	B	475	GLU	N-CA-C	5.58	117.73	108.20
2	B	221	GLN	CA-C-N	5.54	125.45	119.85
2	B	221	GLN	C-N-CA	5.54	125.45	119.85
2	B	315	ASN	N-CA-C	5.51	116.97	111.07
1	A	150	GLU	N-CA-C	5.48	117.25	111.28
2	B	126	VAL	N-CA-C	-5.44	101.71	108.89
2	B	539	VAL	CB-CA-C	-5.39	104.05	111.65
2	B	474	ASN	N-CA-C	5.37	117.55	111.11
2	B	107	ASN	N-CA-C	-5.31	101.81	110.20
2	B	278	THR	N-CA-C	-5.25	102.22	110.36
1	A	195	TYR	N-CA-C	5.18	118.00	109.76
1	A	166	GLU	N-CA-C	5.15	116.58	111.07
2	B	318	LYS	N-CA-C	-5.05	105.66	111.07
2	B	312	SER	N-CA-C	5.03	117.50	111.71
2	B	229	VAL	CB-CA-C	-5.01	102.03	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	196	TYR	Sidechain

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	1609	0	1519	43	0
2	B	4408	0	4202	99	0
3	A	10	0	0	0	0
3	B	10	0	0	2	0
4	B	1	0	0	0	0
5	A	201	0	0	4	0
5	B	575	0	0	8	0
All	All	6814	0	5721	126	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 11.

All (126) 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)
2:B:277:LEU:HD22	2:B:282:MET:HE2	1.46	0.94
1:A:136:MET:SD	2:B:151:LEU:HD13	2.14	0.87
1:A:11:ASN:H	1:A:11:ASN:HD22	1.21	0.86
2:B:112:GLN:HE21	2:B:112:GLN:HA	1.49	0.77
2:B:535:ASN:O	2:B:539:VAL:HG23	1.89	0.72
2:B:533:TRP:HB3	2:B:539:VAL:HG22	1.72	0.72
2:B:332:LEU:HD22	2:B:475:GLU:HB2	1.71	0.71
1:A:188:ILE:HG12	2:B:229:VAL:CG2	2.24	0.68
1:A:11:ASN:HD22	1:A:11:ASN:N	1.90	0.68
1:A:136:MET:CE	2:B:151:LEU:HD13	2.24	0.68
1:A:161:LYS:HG2	1:A:166:GLU:HA	1.77	0.67
2:B:127:VAL:HG21	2:B:139:LYS:HE3	1.76	0.66
1:A:136:MET:HE1	2:B:151:LEU:HD13	1.78	0.66
2:B:440:ASP:O	2:B:442:PRO:HD3	1.95	0.65
2:B:380:GLN:HG3	2:B:381:GLU:HG3	1.78	0.64
1:A:5:ILE:HD11	2:B:551:ILE:HD13	1.80	0.64
1:A:92:ARG:NH2	1:A:129:SER:H	1.97	0.63
2:B:378:THR:HG22	2:B:379:THR:H	1.65	0.61
1:A:116:GLN:HG3	2:B:466:LEU:HG	1.83	0.61
1:A:167:GLN:O	1:A:171:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:SD	2:B:151:LEU:HD22	2.42	0.59
1:A:107:THR:HG22	1:A:108:LYS:N	2.16	0.59
2:B:201:ILE:O	2:B:202:ASN:HB2	2.03	0.59
2:B:253:LEU:HD22	5:B:1106:HOH:O	2.02	0.59
1:A:143:ARG:HD3	1:A:144:PHE:CE2	2.36	0.58
2:B:433:LYS:O	2:B:437:LYS:HG3	2.04	0.58
2:B:539:VAL:HG12	2:B:543:ILE:HD11	1.86	0.58
2:B:378:THR:HG22	2:B:379:THR:N	2.18	0.57
2:B:380:GLN:HG3	2:B:381:GLU:N	2.18	0.57
2:B:277:LEU:HD22	2:B:282:MET:CE	2.26	0.57
2:B:419:GLN:O	2:B:423:ILE:HG13	2.05	0.57
1:A:11:ASN:H	1:A:11:ASN:ND2	1.99	0.56
2:B:297:ARG:HD2	5:B:828:HOH:O	2.05	0.56
2:B:8:LYS:HE2	5:B:780:HOH:O	2.06	0.55
2:B:112:GLN:HB2	5:B:1118:HOH:O	2.06	0.55
1:A:136:MET:SD	2:B:151:LEU:CD1	2.93	0.55
2:B:99:MET:HG2	2:B:121:THR:HG22	1.88	0.55
1:A:108:LYS:O	1:A:108:LYS:HG3	2.08	0.54
1:A:8:GLU:OE1	2:B:546:THR:HG23	2.07	0.54
2:B:359:LEU:HD13	2:B:371:TYR:HB3	1.91	0.53
2:B:2:ASN:HA	2:B:239:ASN:O	2.09	0.53
1:A:27:TYR:HA	1:A:93:GLY:O	2.09	0.52
2:B:5:LEU:HG	2:B:18:LEU:HD22	1.91	0.52
2:B:533:TRP:CB	2:B:539:VAL:HG22	2.39	0.52
1:A:16:HIS:HD2	2:B:38:HIS:NE2	2.07	0.52
5:A:917:HOH:O	2:B:127:VAL:HG23	2.08	0.52
2:B:451:ALA:HB1	2:B:472:HIS:CE1	2.44	0.52
1:A:188:ILE:HG12	2:B:229:VAL:HG22	1.92	0.52
2:B:456:GLU:HB2	2:B:465:ALA:HB3	1.91	0.52
2:B:379:THR:HG22	2:B:380:GLN:H	1.75	0.51
1:A:136:MET:HG2	2:B:52:TYR:CD1	2.46	0.51
2:B:316:SER:HB3	2:B:428:ASN:OD1	2.11	0.51
2:B:332:LEU:HD21	2:B:474:ASN:HB3	1.93	0.50
1:A:5:ILE:CD1	2:B:551:ILE:HD13	2.41	0.50
2:B:103:GLN:HE22	2:B:117:GLU:CD	2.20	0.50
5:A:917:HOH:O	2:B:127:VAL:CG2	2.60	0.49
2:B:265:LYS:HB2	2:B:297:ARG:NH2	2.28	0.49
2:B:380:GLN:HG3	2:B:381:GLU:H	1.76	0.49
2:B:151:LEU:HD12	2:B:151:LEU:O	2.13	0.49
2:B:383:PRO:HD3	2:B:450:THR:CG2	2.43	0.49
1:A:19:ALA:O	2:B:39:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.48	0.49
2:B:401:LEU:HG	2:B:404:LYS:HB2	1.95	0.48
1:A:74:ASP:OD1	1:A:78:LYS:HE3	2.13	0.48
1:A:92:ARG:NH1	5:A:842:HOH:O	2.45	0.48
2:B:36:GLY:HA2	2:B:44:ILE:O	2.14	0.48
2:B:426:THR:HG22	5:B:940:HOH:O	2.13	0.48
2:B:454:PHE:O	2:B:470:ASN:HB2	2.14	0.48
2:B:197:PRO:HG2	2:B:199:ARG:CZ	2.44	0.48
2:B:112:GLN:HA	2:B:112:GLN:NE2	2.25	0.47
2:B:504:SER:O	2:B:517:TYR:HA	2.13	0.47
2:B:540:ALA:HB3	2:B:541:PRO:HD3	1.96	0.47
1:A:75:SER:O	1:A:79:GLN:HG3	2.15	0.47
1:A:41:MET:HE1	5:B:571:HOH:O	2.15	0.47
2:B:104:GLU:O	2:B:115:THR:HA	2.15	0.47
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.50	0.47
1:A:71:TYR:CE2	1:A:134:MET:HE2	2.50	0.47
1:A:92:ARG:HH22	1:A:129:SER:H	1.62	0.46
2:B:56:LEU:HD22	2:B:154:TRP:CE2	2.51	0.46
1:A:108:LYS:HE3	1:A:111:ASP:HB2	1.98	0.46
2:B:9:THR:O	2:B:276:LYS:HE2	2.16	0.45
2:B:281:ASP:O	2:B:284:ALA:HB3	2.16	0.45
1:A:13:GLY:HA3	2:B:516:HIS:CD2	2.51	0.45
2:B:166:TRP:CZ2	2:B:179:TRP:HB3	2.51	0.45
2:B:2:ASN:C	2:B:2:ASN:HD22	2.25	0.45
2:B:316:SER:O	2:B:320:VAL:HG23	2.16	0.44
2:B:17:ILE:HG23	2:B:487:VAL:HG22	2.00	0.44
1:A:39:PHE:CZ	1:A:120:TYR:CD2	3.05	0.44
1:A:151:ILE:O	1:A:154:LEU:HB3	2.17	0.44
2:B:173:GLN:HG3	2:B:179:TRP:CZ2	2.53	0.44
2:B:243:SER:HA	2:B:244:PRO:HD3	1.85	0.44
2:B:458:ASN:OD1	2:B:460:PHE:HB2	2.18	0.44
1:A:92:ARG:HD2	5:A:867:HOH:O	2.17	0.44
1:A:161:LYS:HA	1:A:169:GLY:HA3	1.99	0.44
2:B:25:GLY:HA2	2:B:384:THR:O	2.17	0.44
2:B:401:LEU:O	2:B:404:LYS:HE3	2.17	0.44
2:B:331:GLN:HB2	2:B:340:ILE:HG12	2.00	0.43
2:B:250:ALA:HB2	2:B:258:TRP:CE3	2.54	0.43
2:B:472:HIS:HB2	5:B:700:HOH:O	2.18	0.43
1:A:181:ASN:HA	1:A:182:PRO:HD3	1.87	0.43
2:B:64:SER:OG	2:B:182:ALA:HB3	2.19	0.43
2:B:261:ALA:HB2	2:B:397:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ILE:HG13	2:B:36:GLY:N	2.34	0.43
2:B:151:LEU:HD12	2:B:151:LEU:C	2.43	0.42
2:B:82:VAL:HG13	2:B:87:PRO:HA	2.02	0.42
2:B:301:PRO:O	2:B:305:GLN:HG2	2.19	0.42
1:A:23:TYR:CE1	1:A:93:GLY:HA2	2.55	0.42
2:B:363:VAL:O	2:B:368:ASP:HB3	2.20	0.41
2:B:368:ASP:N	2:B:368:ASP:OD1	2.53	0.41
2:B:376:TYR:O	2:B:378:THR:N	2.53	0.41
2:B:441:ASN:HB3	3:B:556:SO4:O3	2.21	0.41
1:A:65:LYS:O	1:A:69:ASN:HB2	2.20	0.41
1:A:104:GLN:O	1:A:107:THR:HB	2.20	0.41
2:B:148:LEU:N	2:B:148:LEU:HD22	2.36	0.41
2:B:444:ASN:ND2	3:B:556:SO4:O4	2.54	0.41
1:A:71:TYR:CE2	1:A:73:PRO:HG3	2.56	0.41
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.88	0.41
2:B:65:TRP:HA	2:B:180:TYR:O	2.21	0.41
2:B:8:LYS:HE3	5:B:1028:HOH:O	2.21	0.40
2:B:103:GLN:HE22	2:B:117:GLU:CG	2.34	0.40
2:B:2:ASN:HB3	2:B:240:TRP:CD1	2.57	0.40
2:B:23:GLN:HG3	2:B:480:GLY:HA2	2.02	0.40
2:B:86:ASP:OD2	2:B:89:SER:HB2	2.22	0.40
2:B:397:TYR:O	2:B:401:LEU:HB2	2.21	0.40
1:A:113:MET:O	2:B:509:PRO:HG3	2.21	0.40
2:B:337:LYS:HA	2:B:337:LYS:HD3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	195/205 (95%)	188 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	551/553 (100%)	533 (97%)	17 (3%)	1 (0%)	43	63
All	All	746/758 (98%)	721 (97%)	24 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	377	GLU

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	175/183 (96%)	165 (94%)	10 (6%)	18	39
2	B	468/468 (100%)	441 (94%)	27 (6%)	18	38
All	All	643/651 (99%)	606 (94%)	37 (6%)	18	38

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	11	ASN
1	A	107	THR
1	A	140	LEU
1	A	145	SER
1	A	147	MET
1	A	163	LYS
1	A	166	GLU
1	A	179	LEU
1	A	196	SER
2	B	2	ASN
2	B	5	LEU
2	B	18	LEU
2	B	53	PRO
2	B	56	LEU

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Mol	Chain	Res	Type
2	B	82	VAL
2	B	112	GLN
2	B	127	VAL
2	B	132	THR
2	B	149	THR
2	B	151	LEU
2	B	154	TRP
2	B	155	VAL
2	B	184	LYS
2	B	201	ILE
2	B	209	VAL
2	B	229	VAL
2	B	298	LEU
2	B	351	LEU
2	B	369	LYS
2	B	379	THR
2	B	387	LEU
2	B	395	LEU
2	B	396	LEU
2	B	413	LEU
2	B	436	GLU
2	B	529	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	20	ASN
1	A	86	GLN
2	B	2	ASN
2	B	62	HIS
2	B	103	GLN
2	B	107	ASN
2	B	112	GLN
2	B	134	HIS
2	B	202	ASN
2	B	241	ASN
2	B	287	GLN
2	B	295	ASN
2	B	361	GLN
2	B	420	ASN

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Mol	Chain	Res	Type
2	B	473	GLN
2	B	525	GLN
2	B	526	GLN
2	B	535	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	2.43	1 (14%)	9,10,12	1.61	2 (22%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	6.00	1.49	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-CG	-2.99	121.38	126.72
1	A	1	PCA	OE-CD-N	-2.33	119.91	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
3	SO4	A	255	-	4,4,4	0.31	0	6,6,6	0.45	0
3	SO4	A	269	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	B	556	-	4,4,4	0.87	0	6,6,6	0.31	0
3	SO4	B	555	-	4,4,4	0.47	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	556	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.