



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:13 PM UTC

PDB ID : 2AZQ / pdb_00002azq
Title : Crystal Structure of Catechol 1,2-Dioxygenase from Pseudomonas arvilla C-1
Authors : Earhart, C.A.; Vetting, M.W.; Gosu, R.; Michaud-Soret, I.; Que, L.; Ohlen-
dorf, D.H.
Deposited on : 2005-09-12
Resolution : 2.65 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

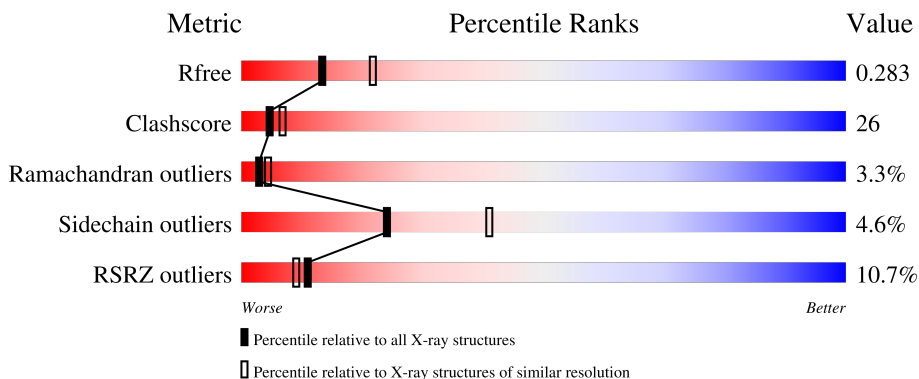
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	311	11% 55% 36% 6% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2456 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 catechol 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2411	1509	440	458	4			

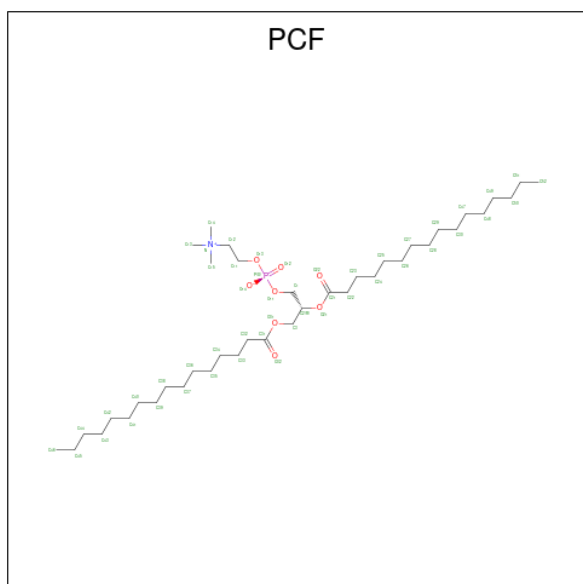
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	PHE	PRO	conflict	UNP Q51433
A	299	ALA	GLU	conflict	UNP Q51433

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).

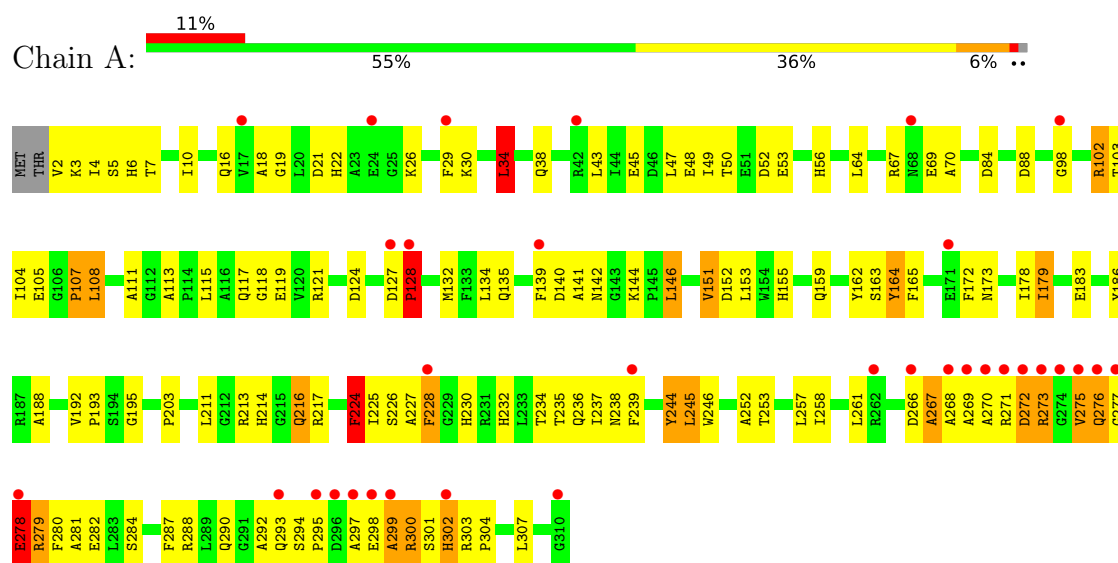


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

3 Residue-property plots [i](#)

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

- Molecule 1: catechol 1,2-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	62.73Å 71.52Å 187.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.65 21.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	84.4 (21.00-2.65) 84.1 (21.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.284 0.229 , 0.283	Depositor DCC
R_{free} test set	555 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2456	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.76	0/2465	1.26	27/3335 (0.8%)

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
1	A	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	GLY	N-CA-C	9.63	125.26	110.91
1	A	67	ARG	N-CA-C	-9.11	102.18	113.38
1	A	127	ASP	CA-C-N	8.05	129.90	119.84
1	A	127	ASP	C-N-CA	8.05	129.90	119.84
1	A	108	LEU	N-CA-C	7.72	122.45	112.26
1	A	195	GLY	N-CA-C	-6.95	101.88	112.51
1	A	224	PHE	N-CA-C	-6.55	97.73	108.41
1	A	34	LEU	N-CA-C	-6.54	104.15	111.28
1	A	213	ARG	N-CA-C	6.50	120.49	110.42
1	A	159	GLN	N-CA-C	-6.32	105.53	113.18
1	A	295	PRO	N-CA-C	-6.25	105.39	113.57
1	A	127	ASP	N-CA-C	6.19	119.11	110.07
1	A	302	HIS	N-CA-C	-6.18	105.60	113.02
1	A	301	SER	N-CA-C	-6.09	102.92	110.41
1	A	278	GLU	N-CA-C	5.98	123.54	110.80
1	A	237	ILE	N-CA-C	-5.96	99.05	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	HIS	N-CA-C	5.86	116.29	108.38
1	A	153	LEU	N-CA-C	5.80	118.67	109.50
1	A	307	LEU	N-CA-C	5.79	121.60	113.56
1	A	244	TYR	N-CA-C	5.66	120.17	113.16
1	A	121	ARG	N-CA-C	-5.65	100.50	109.76
1	A	165	PHE	N-CA-C	-5.54	105.64	112.90
1	A	128	PRO	N-CA-C	-5.49	101.17	112.47
1	A	179	ILE	CB-CA-C	-5.41	104.20	110.91
1	A	43	LEU	CA-CB-CG	5.24	134.62	116.30
1	A	273	ARG	N-CA-C	5.20	120.49	113.21
1	A	111	ALA	N-CA-C	5.02	117.16	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	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	2411	0	2299	121	1
2	A	1	0	0	0	0
3	A	44	0	65	4	0
All	All	2456	0	2364	125	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (125) 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:261:LEU:HD11	1:A:281:ALA:HB1	1.25	1.15
3:A:954:PCF:H331	3:A:954:PCF:H32	1.28	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:H	1:A:228:PHE:HD1	1.11	0.97
1:A:98:GLY:HA3	1:A:290:GLN:NE2	1.80	0.96
1:A:214:HIS:HD2	1:A:216:GLN:H	1.05	0.91
1:A:102:ARG:HH21	1:A:102:ARG:HG3	1.38	0.89
1:A:275:VAL:HG12	1:A:276:GLN:H	1.39	0.88
1:A:132:MET:HE3	1:A:192:VAL:HA	1.58	0.84
1:A:214:HIS:CD2	1:A:216:GLN:H	1.93	0.84
1:A:278:GLU:O	1:A:279:ARG:HB2	1.77	0.83
1:A:98:GLY:HA3	1:A:290:GLN:HE21	1.46	0.78
1:A:34:LEU:HD22	1:A:38:GLN:HE21	1.48	0.78
1:A:152:ASP:HB3	1:A:224:PHE:HB2	1.63	0.78
1:A:226:SER:HB2	1:A:298:GLU:HG3	1.70	0.74
1:A:273:ARG:NH1	1:A:282:GLU:OE1	2.22	0.72
3:A:954:PCF:H331	3:A:954:PCF:C3	2.14	0.71
1:A:84:ASP:HB3	1:A:102:ARG:HD3	1.73	0.71
1:A:214:HIS:HD2	1:A:216:GLN:N	1.87	0.70
1:A:115:LEU:HD11	1:A:179:ILE:HD11	1.74	0.69
1:A:271:ARG:O	1:A:272:ASP:HB2	1.94	0.68
1:A:102:ARG:HG3	1:A:102:ARG:NH2	2.09	0.67
1:A:98:GLY:CA	1:A:290:GLN:NE2	2.58	0.67
1:A:228:PHE:CD1	1:A:228:PHE:N	2.59	0.67
1:A:34:LEU:HD22	1:A:38:GLN:NE2	2.09	0.66
1:A:132:MET:CE	1:A:192:VAL:HA	2.27	0.65
1:A:238:ASN:ND2	1:A:253:THR:HG22	2.12	0.65
1:A:4:ILE:O	1:A:7:THR:HG23	1.97	0.64
1:A:278:GLU:O	1:A:279:ARG:CB	2.45	0.63
1:A:232:HIS:HB2	1:A:298:GLU:HA	1.80	0.62
1:A:245:LEU:O	1:A:253:THR:HG21	1.99	0.62
1:A:26:LYS:HD2	1:A:29:PHE:CE1	2.35	0.62
1:A:299:ALA:O	1:A:300:ARG:O	2.18	0.62
1:A:146:LEU:HD21	1:A:230:HIS:NE2	2.15	0.61
1:A:267:ALA:HA	1:A:278:GLU:H	1.64	0.61
1:A:275:VAL:HG12	1:A:276:GLN:N	2.13	0.61
3:A:954:PCF:C3	3:A:954:PCF:C33	2.77	0.61
1:A:266:ASP:O	1:A:267:ALA:C	2.45	0.59
1:A:246:TRP:CZ2	1:A:258:ILE:HD11	2.37	0.59
3:A:954:PCF:H32	3:A:954:PCF:C33	2.10	0.59
1:A:3:LYS:O	1:A:6:HIS:HE1	1.87	0.58
1:A:238:ASN:CG	1:A:253:THR:HG22	2.28	0.58
1:A:47:LEU:HB2	1:A:49:ILE:CD1	2.33	0.57
1:A:64:LEU:HD21	1:A:70:ALA:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PHE:HE1	1:A:282:GLU:CG	2.17	0.57
1:A:69:GLU:OE1	1:A:203:PRO:HD2	2.04	0.57
1:A:124:ASP:H	1:A:173:ASN:HD21	1.53	0.57
1:A:280:PHE:HE1	1:A:282:GLU:HG3	1.70	0.57
1:A:48:GLU:HG2	1:A:48:GLU:O	2.04	0.56
1:A:266:ASP:C	1:A:266:ASP:OD2	2.48	0.56
1:A:4:ILE:HG13	1:A:10:ILE:HG13	1.88	0.56
1:A:135:GLN:O	1:A:284:SER:HA	2.06	0.56
1:A:98:GLY:HA2	1:A:290:GLN:HG2	1.88	0.55
1:A:146:LEU:HD21	1:A:230:HIS:CD2	2.42	0.55
1:A:266:ASP:OD2	1:A:268:ALA:N	2.39	0.55
1:A:140:ASP:OD1	1:A:144:LYS:HB2	2.07	0.54
1:A:49:ILE:HG23	1:A:53:GLU:HB2	1.90	0.53
1:A:178:ILE:HG21	1:A:186:TYR:HB2	1.89	0.53
1:A:292:ALA:HB1	1:A:297:ALA:CB	2.38	0.53
1:A:280:PHE:CE1	1:A:282:GLU:HG3	2.44	0.53
1:A:269:ALA:N	1:A:276:GLN:O	2.42	0.52
1:A:183:GLU:O	1:A:183:GLU:HG2	2.09	0.52
1:A:267:ALA:CA	1:A:278:GLU:H	2.21	0.52
1:A:132:MET:HE2	1:A:239:PHE:HE2	1.75	0.52
1:A:225:ILE:HD12	1:A:287:PHE:CG	2.45	0.52
1:A:132:MET:HE2	1:A:239:PHE:CE2	2.45	0.52
1:A:226:SER:HB2	1:A:298:GLU:CG	2.39	0.52
1:A:50:THR:OG1	1:A:53:GLU:HG3	2.10	0.51
1:A:155:HIS:ND1	1:A:193:PRO:HB3	2.25	0.51
1:A:18:ALA:O	1:A:30:LYS:HG2	2.10	0.51
1:A:140:ASP:OD2	1:A:142:ASN:N	2.44	0.51
1:A:134:LEU:HB3	1:A:188:ALA:HB3	1.93	0.51
1:A:3:LYS:O	1:A:6:HIS:CE1	2.64	0.50
1:A:163:SER:O	1:A:164:TYR:HB3	2.10	0.50
1:A:52:ASP:O	1:A:56:HIS:HD2	1.94	0.50
1:A:132:MET:HE1	1:A:193:PRO:HD2	1.93	0.50
1:A:266:ASP:O	1:A:268:ALA:N	2.45	0.49
1:A:132:MET:HE1	1:A:193:PRO:CD	2.42	0.49
1:A:19:GLY:C	1:A:21:ASP:H	2.19	0.49
1:A:16:GLN:O	1:A:21:ASP:OD1	2.31	0.49
1:A:98:GLY:HA2	1:A:290:GLN:CG	2.42	0.48
1:A:239:PHE:CD1	1:A:239:PHE:N	2.81	0.48
1:A:271:ARG:O	1:A:272:ASP:CB	2.61	0.48
1:A:140:ASP:OD2	1:A:140:ASP:C	2.56	0.48
1:A:292:ALA:HB1	1:A:297:ALA:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HB2	1:A:49:ILE:HD11	1.96	0.47
1:A:107:PRO:HG2	1:A:108:LEU:HG	1.96	0.47
1:A:5:SER:HB3	1:A:45:GLU:OE2	2.15	0.46
1:A:293:GLN:O	1:A:294:SER:HB3	2.16	0.46
1:A:268:ALA:C	1:A:270:ALA:H	2.24	0.45
1:A:230:HIS:C	1:A:292:ALA:HB2	2.41	0.45
1:A:64:LEU:HD12	1:A:203:PRO:HB2	1.99	0.45
1:A:88:ASP:OD2	1:A:102:ARG:NE	2.46	0.45
1:A:117:GLN:O	1:A:119:GLU:N	2.41	0.45
1:A:217:ARG:NH2	1:A:236:GLN:OE1	2.49	0.45
1:A:105:GLU:HB2	1:A:234:THR:HG21	1.99	0.44
1:A:239:PHE:N	1:A:239:PHE:HD1	2.15	0.44
1:A:50:THR:HG23	1:A:53:GLU:OE1	2.18	0.44
1:A:141:ALA:O	1:A:288:ARG:NH2	2.49	0.43
1:A:225:ILE:HD12	1:A:287:PHE:CD2	2.53	0.43
1:A:113:ALA:HA	1:A:172:PHE:CD2	2.54	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.81	0.43
1:A:34:LEU:O	1:A:38:GLN:HG3	2.19	0.43
1:A:151:VAL:HG22	1:A:151:VAL:O	2.18	0.43
1:A:155:HIS:HD1	1:A:193:PRO:HB3	1.83	0.43
1:A:299:ALA:C	1:A:300:ARG:O	2.61	0.43
1:A:163:SER:O	1:A:164:TYR:CB	2.68	0.42
1:A:19:GLY:O	1:A:30:LYS:HE2	2.19	0.42
1:A:214:HIS:CD2	1:A:214:HIS:C	2.97	0.42
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.87	0.42
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.79	0.42
1:A:104:ILE:HG12	1:A:252:ALA:HB2	2.01	0.42
1:A:139:PHE:C	1:A:146:LEU:HD12	2.45	0.42
1:A:217:ARG:HH22	1:A:236:GLN:CD	2.27	0.42
1:A:103:THR:HG22	1:A:235:THR:HA	2.01	0.42
1:A:272:ASP:O	1:A:273:ARG:HG3	2.20	0.42
1:A:298:GLU:O	1:A:299:ALA:HB2	2.21	0.41
1:A:280:PHE:CD1	1:A:280:PHE:C	2.97	0.41
1:A:302:HIS:O	1:A:303:ARG:C	2.60	0.41
1:A:128:PRO:O	1:A:128:PRO:HG2	2.20	0.41
1:A:244:TYR:O	1:A:245:LEU:C	2.63	0.41
1:A:98:GLY:CA	1:A:290:GLN:CD	2.94	0.41
1:A:108:LEU:HD13	1:A:162:TYR:CD1	2.56	0.41
1:A:227:ALA:O	1:A:228:PHE:C	2.63	0.40
1:A:151:VAL:O	1:A:151:VAL:CG2	2.68	0.40
1:A:303:ARG:HA	1:A:304:PRO:HD3	1.88	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:NH2	1:A:273:ARG:NH2[3_654]	1.35	0.85

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	307/311 (99%)	275 (90%)	22 (7%)	10 (3%)	3 4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	A	278	GLU
1	A	128	PRO
1	A	272	ASP
1	A	279	ARG
1	A	299	ALA
1	A	300	ARG
1	A	276	GLN
1	A	267	ALA
1	A	275	VAL

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	240/242 (99%)	229 (95%)	11 (5%)	24	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	34	LEU
1	A	102	ARG
1	A	107	PRO
1	A	128	PRO
1	A	146	LEU
1	A	151	VAL
1	A	216	GLN
1	A	224	PHE
1	A	228	PHE
1	A	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	15	ASN
1	A	38	GLN
1	A	56	HIS
1	A	68	ASN
1	A	81	HIS
1	A	137	GLN
1	A	173	ASN
1	A	205	GLN
1	A	214	HIS
1	A	238	ASN
1	A	290	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PCF	A	954	-	43,43,49	0.74	0	49,51,57	1.34	4 (8%)

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
3	PCF	A	954	-	-	17/47/47/53	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	954	PCF	O21-C21-C22	6.18	124.85	111.48
3	A	954	PCF	O21-C21-O22	-2.93	116.84	123.70
3	A	954	PCF	C39-C38-C37	-2.29	102.81	114.37
3	A	954	PCF	C23-C22-C21	-2.10	106.00	113.69

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	954	PCF	O32-C31-O31-C3
3	A	954	PCF	C32-C31-O31-C3

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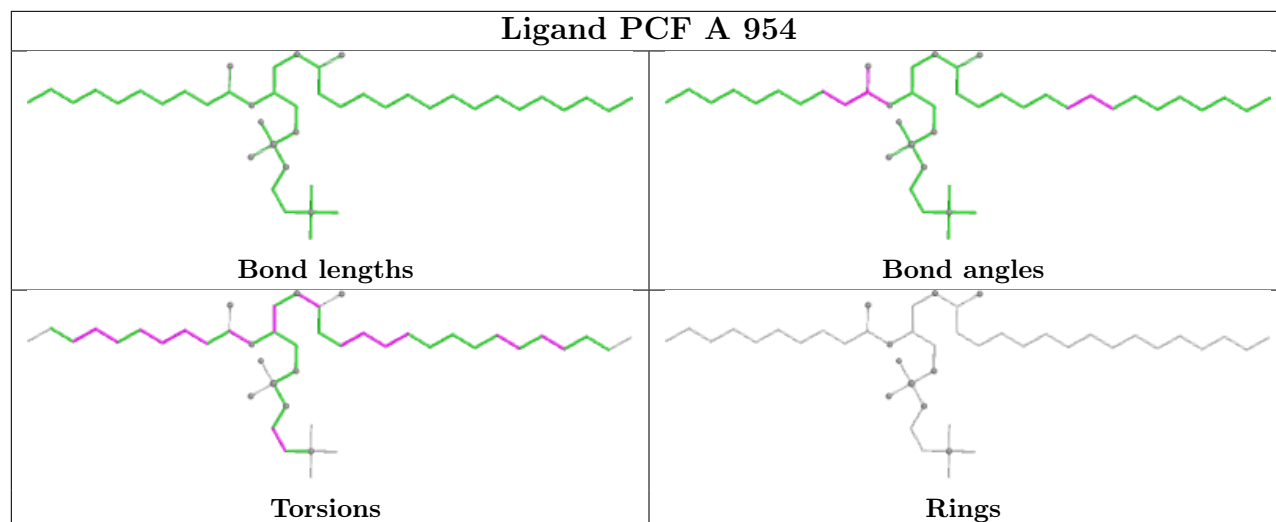
Mol	Chain	Res	Type	Atoms
3	A	954	PCF	O22-C21-O21-C2
3	A	954	PCF	C22-C21-O21-C2
3	A	954	PCF	C21-C22-C23-C24
3	A	954	PCF	C25-C26-C27-C28
3	A	954	PCF	C33-C34-C35-C36
3	A	954	PCF	C34-C35-C36-C37
3	A	954	PCF	O13-C11-C12-N
3	A	954	PCF	C23-C24-C25-C26
3	A	954	PCF	C22-C23-C24-C25
3	A	954	PCF	C41-C42-C43-C44
3	A	954	PCF	O21-C2-C3-O31
3	A	954	PCF	C32-C33-C34-C35
3	A	954	PCF	C26-C27-C28-C29
3	A	954	PCF	C1-C2-C3-O31
3	A	954	PCF	C39-C40-C41-C42

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	954	PCF	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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	309/311 (99%)	0.23	33 (10%) 11 9	2, 11, 44, 66	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	ASP	7.0
1	A	270	ALA	6.7
1	A	275	VAL	5.6
1	A	302	HIS	5.0
1	A	277	GLY	4.4
1	A	268	ALA	4.2
1	A	171	GLU	4.1
1	A	298	GLU	4.1
1	A	276	GLN	3.9
1	A	271	ARG	3.9
1	A	228	PHE	3.6
1	A	269	ALA	3.6
1	A	295	PRO	3.3
1	A	262	ARG	3.2
1	A	293	GLN	3.0
1	A	68	ASN	3.0
1	A	278	GLU	2.8
1	A	266	ASP	2.8
1	A	296	ASP	2.8
1	A	239	PHE	2.8
1	A	299	ALA	2.7
1	A	24	GLU	2.6
1	A	29	PHE	2.5
1	A	139	PHE	2.5
1	A	128	PRO	2.5
1	A	274	GLY	2.4
1	A	297	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	127	ASP	2.3
1	A	42	ARG	2.2
1	A	17	VAL	2.2
1	A	310	GLY	2.2
1	A	273	ARG	2.1
1	A	98	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

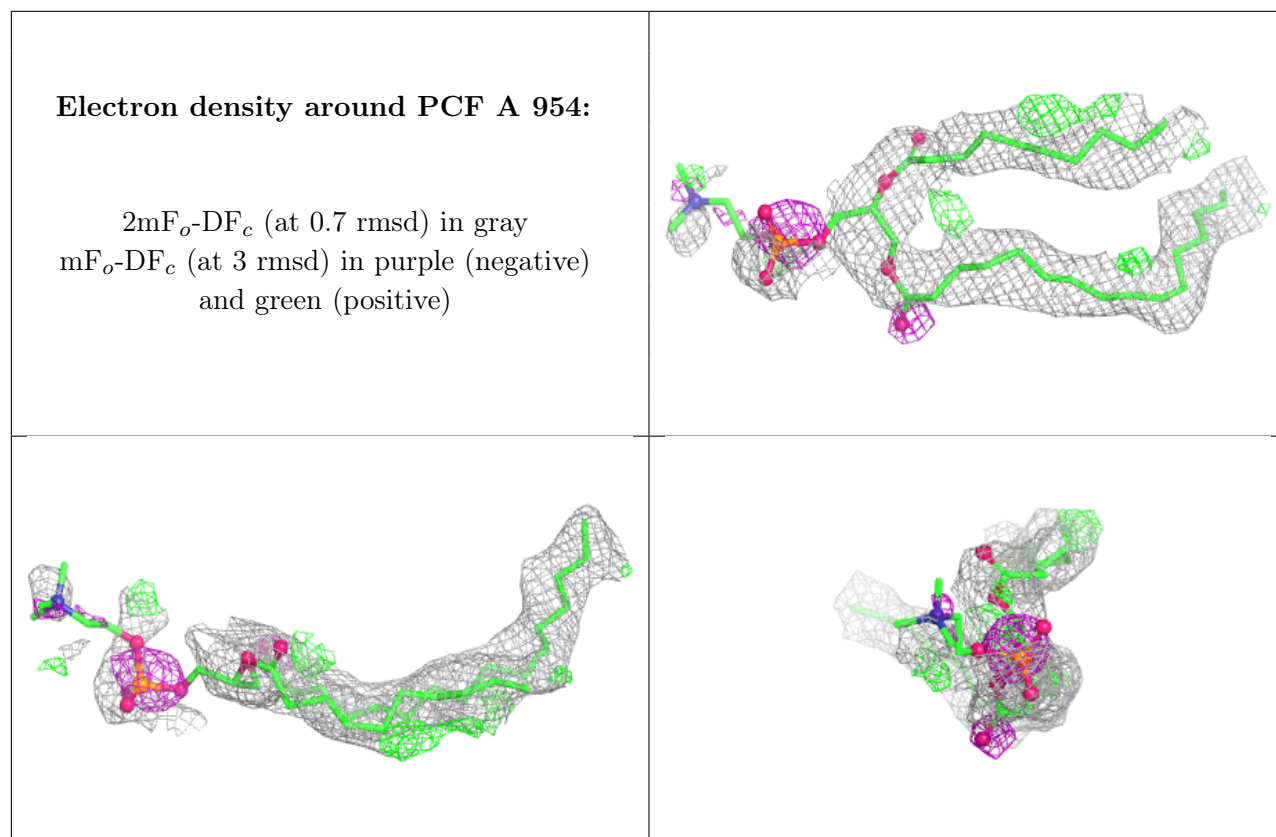
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PCF	A	954	44/50	0.69	0.22	24,38,65,67	0
2	FE	A	400	1/1	0.98	0.05	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.