



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:57 AM UTC

PDB ID : 3PCL / pdb_00003pcl
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 2-HYDROXYISONICOTINIC ACID N-OXIDE AND
CYANIDE
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-18
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

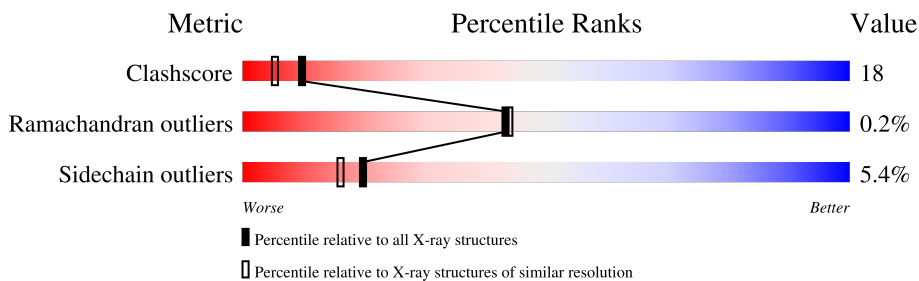
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)





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	200	64% 30% 6%
1	B	200	67% 25% 6% .
1	C	200	63% 31% 6%
1	D	200	65% 29% 6%
1	E	200	57% 34% 8%
1	F	200	53% 36% 10% .
2	M	238	57% 35% 6% .
2	N	238	60% 29% 9% .

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Mol	Chain	Length	Quality of chain
2	O	238	 57% 34% 6% ..
2	P	238	 54% 36% 7% ..
2	Q	238	 54% 32% 10% ..
2	R	238	 53% 35% 8% ..

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	CYN	Q	575	-	-	X	-
3	CYN	R	575	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21960 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.

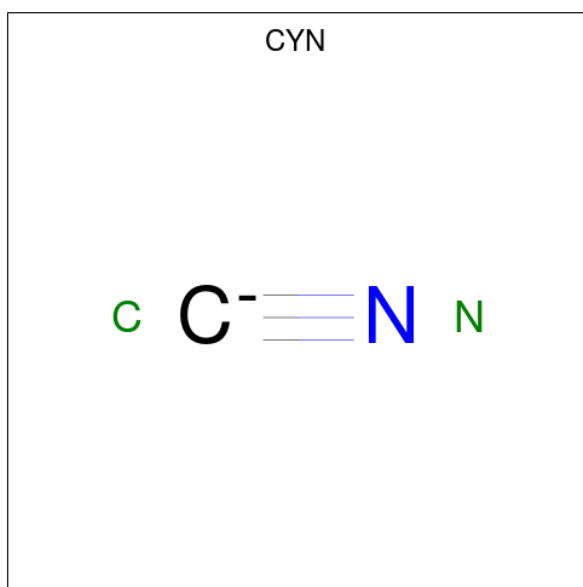
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1571	993	276	299	3	0	0	0
1	B	200	1571	993	276	299	3	0	0	0
1	C	200	1571	993	276	299	3	0	0	0
1	D	200	1571	993	276	299	3	0	0	0
1	E	200	1571	993	276	299	3	0	0	0
1	F	200	1571	993	276	299	3	0	0	0

- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	233	1840	1171	334	328	7	0	0	0
2	N	233	1840	1171	334	328	7	0	0	0
2	O	233	1840	1171	334	328	7	0	0	0
2	P	233	1840	1171	334	328	7	0	0	0
2	Q	233	1840	1171	334	328	7	0	0	0
2	R	233	1840	1171	334	328	7	0	0	0

- Molecule 3 is CYANIDE ION (CCD ID: CYN) (formula: CN).

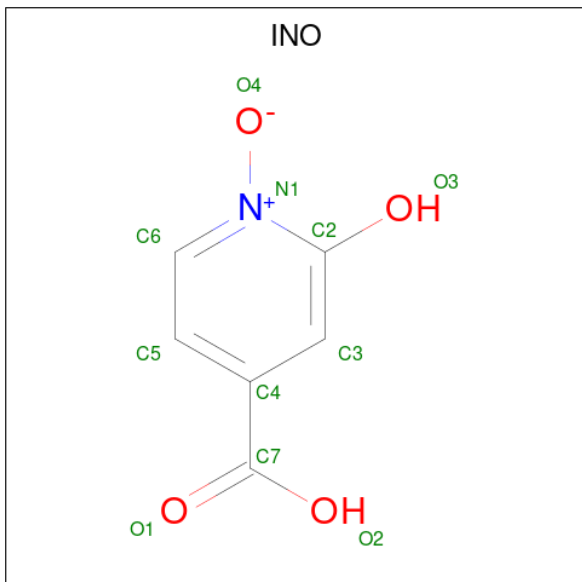


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C N 2 1 1	0	0
3	N	1	Total C N 2 1 1	0	0
3	O	1	Total C N 2 1 1	0	0
3	P	1	Total C N 2 1 1	0	0
3	Q	1	Total C N 2 1 1	0	0
3	R	1	Total C N 2 1 1	0	0

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total Fe 1 1	0	0
4	N	1	Total Fe 1 1	0	0
4	O	1	Total Fe 1 1	0	0
4	P	1	Total Fe 1 1	0	0
4	Q	1	Total Fe 1 1	0	0
4	R	1	Total Fe 1 1	0	0

- Molecule 5 is 2-HYDROXYISONICOTINIC ACID N-OXIDE (CCD ID: INO) (formula: $C_6H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	11	6	1	4	0	0
5	N	1	11	6	1	4	0	0
5	O	1	11	6	1	4	0	0
5	P	1	11	6	1	4	0	0
5	Q	1	11	6	1	4	0	0
5	R	1	11	6	1	4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	76	76	76	0	0
6	M	156	156	156	0	0
6	B	78	78	78	0	0
6	N	159	159	159	0	0

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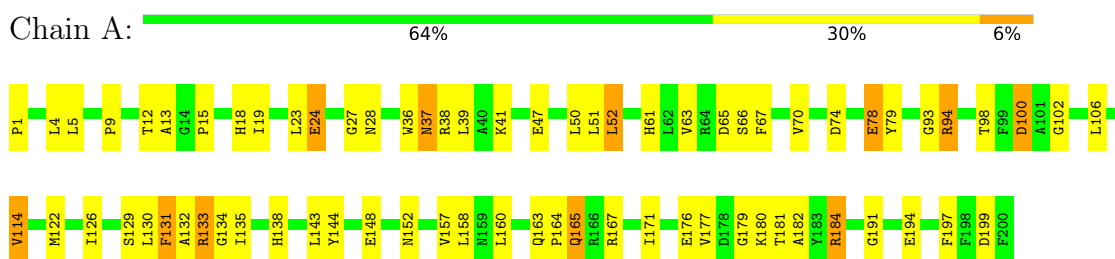
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	79	Total 79	O 79	0	0
6	O	157	Total 157	O 157	0	0
6	D	78	Total 78	O 78	0	0
6	P	152	Total 152	O 152	0	0
6	E	76	Total 76	O 76	0	0
6	Q	165	Total 165	O 165	0	0
6	F	82	Total 82	O 82	0	0
6	R	152	Total 152	O 152	0	0

3 Residue-property plots [i](#)

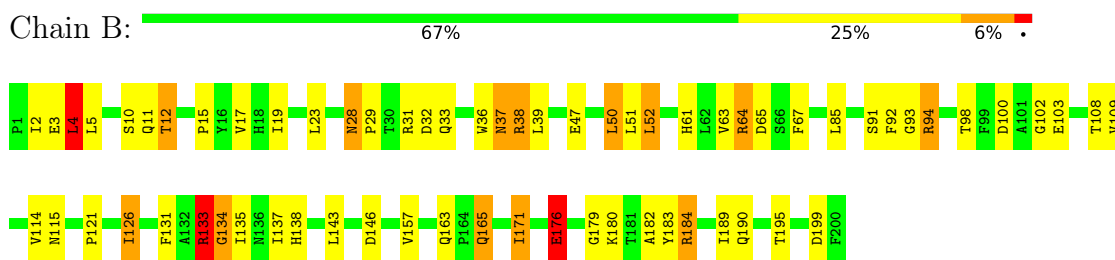
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

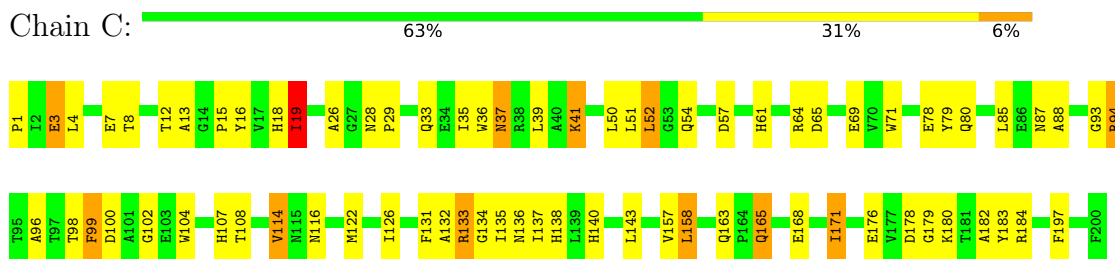
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



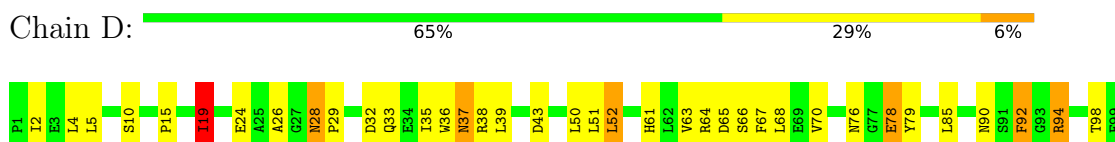
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

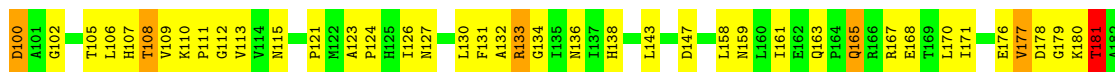
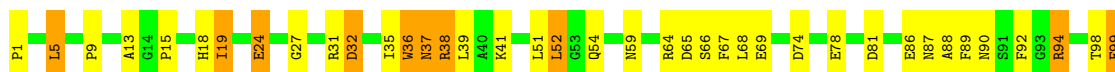


- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

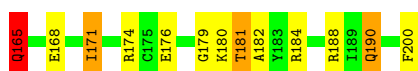
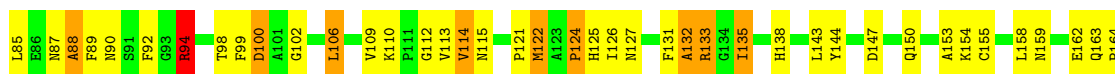
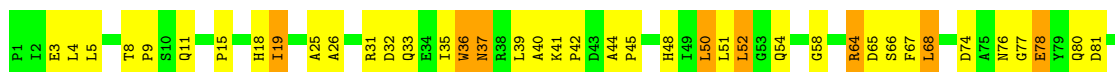




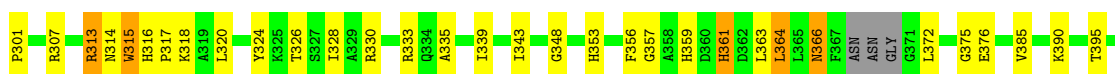
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



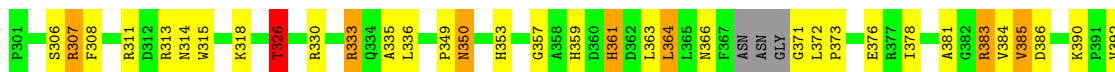
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

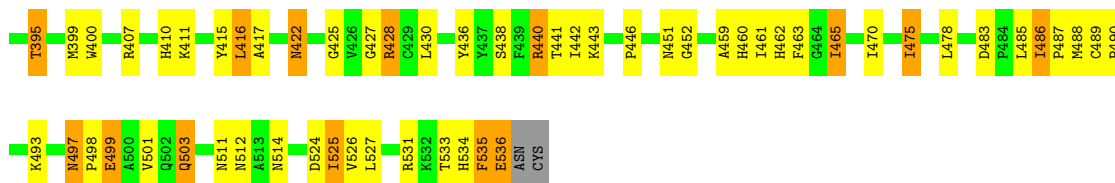


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



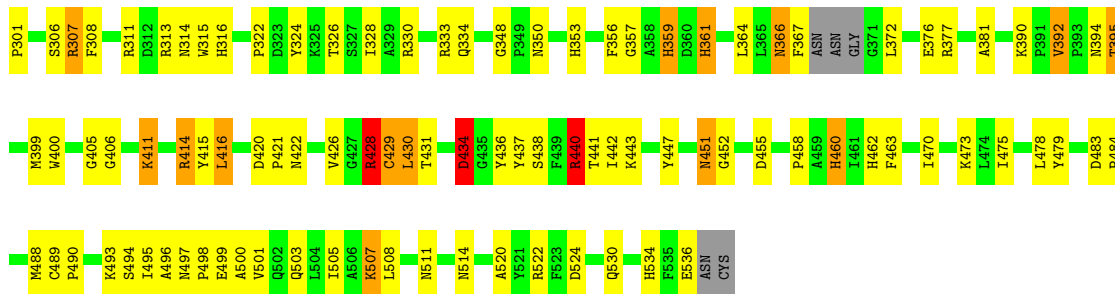
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





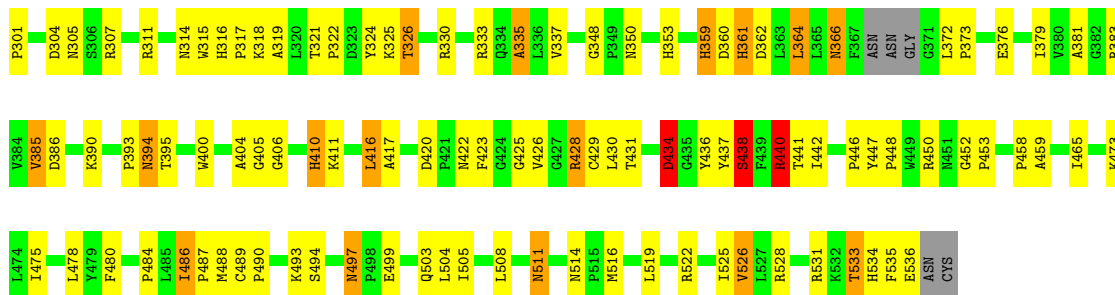
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O: 57% 34% 6% ..



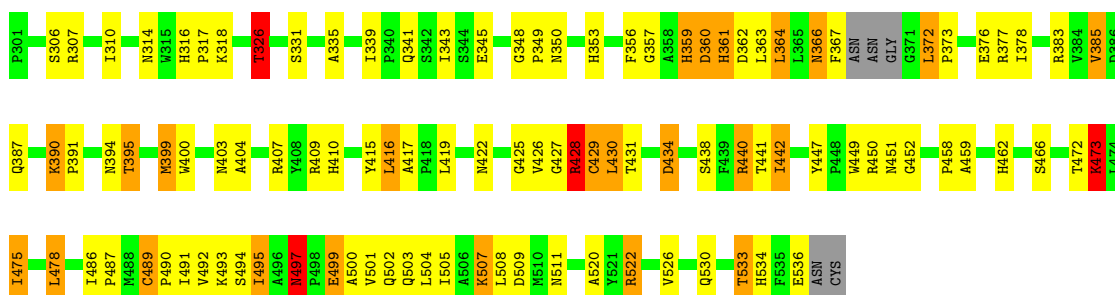
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 54% 36% 7% ..



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 54% 32% 10% ..



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 53% 35% 8% ..

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.70Å 128.00Å 134.20Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	94.0 (6.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	21960	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: FE, CYN, INO

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	1.30	2/1611 (0.1%)	1.86	30/2195 (1.4%)
1	B	1.33	7/1611 (0.4%)	1.92	33/2195 (1.5%)
1	C	1.31	2/1611 (0.1%)	1.86	30/2195 (1.4%)
1	D	1.34	6/1611 (0.4%)	1.81	22/2195 (1.0%)
1	E	1.31	2/1611 (0.1%)	1.84	34/2195 (1.5%)
1	F	1.41	5/1611 (0.3%)	1.88	32/2195 (1.5%)
2	M	1.45	6/1895 (0.3%)	1.93	43/2580 (1.7%)
2	N	1.48	8/1895 (0.4%)	1.95	52/2580 (2.0%)
2	O	1.51	7/1895 (0.4%)	2.00	50/2580 (1.9%)
2	P	1.50	14/1895 (0.7%)	1.95	50/2580 (1.9%)
2	Q	1.49	9/1895 (0.5%)	2.01	59/2580 (2.3%)
2	R	1.49	9/1895 (0.5%)	1.97	46/2580 (1.8%)
All	All	1.42	77/21036 (0.4%)	1.92	481/28650 (1.7%)

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	E	0	1

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	313	ARG	NE-CZ	9.09	1.43	1.33
2	Q	428	ARG	CD-NE	-8.00	1.35	1.46
1	F	135	ILE	CA-CB	7.73	1.62	1.53
2	Q	441	THR	CA-CB	7.22	1.63	1.54
2	O	428	ARG	CD-NE	-7.16	1.36	1.46

The worst 5 of 481 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	428	ARG	CD-NE-CZ	18.09	149.72	124.40
1	A	94	ARG	CD-NE-CZ	16.75	147.86	124.40
1	B	133	ARG	CD-NE-CZ	15.78	146.49	124.40
2	O	428	ARG	CD-NE-CZ	14.94	145.31	124.40
1	B	94	ARG	CD-NE-CZ	14.76	145.06	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	184	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1571	0	1499	49	0
1	B	1571	0	1499	55	0
1	C	1571	0	1499	58	0
1	D	1571	0	1499	57	0
1	E	1571	0	1499	69	0
1	F	1571	0	1499	87	0
2	M	1840	0	1794	68	0
2	N	1840	0	1794	59	0
2	O	1840	0	1794	64	0
2	P	1840	0	1794	81	0
2	Q	1840	0	1794	71	0
2	R	1840	0	1794	75	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	1	0
3	P	2	0	0	1	0
3	Q	2	0	0	2	0
3	R	2	0	0	2	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	M	11	0	3	1	0
5	N	11	0	3	0	0
5	O	11	0	3	0	0
5	P	11	0	3	0	0
5	Q	11	0	3	2	0
5	R	11	0	3	0	0
6	A	76	0	0	2	0
6	B	78	0	0	0	0
6	C	79	0	0	0	0
6	D	78	0	0	0	0
6	E	76	0	0	3	0
6	F	82	0	0	1	0
6	M	156	0	0	6	0
6	N	159	0	0	6	0
6	O	157	0	0	7	0
6	P	152	0	0	8	0
6	Q	165	0	0	8	0
6	R	152	0	0	6	0
All	All	21960	0	19776	711	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 18.

The worst 5 of 711 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:134:GLY:HA3	2:N:326:THR:HG22	1.33	1.07
1:B:165:GLN:H	1:B:165:GLN:NE2	1.52	1.07
1:E:165:GLN:H	1:E:165:GLN:HE21	1.02	1.02
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.44	0.99
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.45	0.96

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	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	B	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	C	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	24	20
1	D	198/200 (99%)	188 (95%)	9 (4%)	1 (0%)	24	20
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	24	20
2	M	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
2	N	229/238 (96%)	221 (96%)	7 (3%)	1 (0%)	30	26
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	30	26
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	10 (4%)	1 (0%)	30	26
All	All	2562/2628 (98%)	2444 (95%)	112 (4%)	6 (0%)	43	44

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	535	PHE
2	N	535	PHE
1	C	132	ALA
1	F	132	ALA
2	R	535	PHE

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	162/163 (99%)	153 (94%)	9 (6%)	19	15
1	B	162/163 (99%)	151 (93%)	11 (7%)	14	10
1	C	162/163 (99%)	157 (97%)	5 (3%)	35	37
1	D	162/163 (99%)	152 (94%)	10 (6%)	16	12
1	E	162/163 (99%)	156 (96%)	6 (4%)	30	30
1	F	162/163 (99%)	152 (94%)	10 (6%)	16	12
2	M	196/202 (97%)	188 (96%)	8 (4%)	27	26
2	N	196/202 (97%)	192 (98%)	4 (2%)	48	54
2	O	196/202 (97%)	183 (93%)	13 (7%)	15	10
2	P	196/202 (97%)	187 (95%)	9 (5%)	24	22
2	Q	196/202 (97%)	179 (91%)	17 (9%)	9	5
2	R	196/202 (97%)	181 (92%)	15 (8%)	12	7
All	All	2148/2190 (98%)	2031 (95%)	117 (5%)	20	16

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	114	VAL
2	R	428	ARG
1	E	52	LEU
2	R	416	LEU
1	F	100	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	80	GLN
2	R	530	GLN
2	P	412	ASN
2	R	497	ASN
1	F	11	GLN

5.3.3 RNA

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](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	CYN	M	575	4	1,1,1	0.44	0	-		
3	CYN	N	575	4	1,1,1	0.42	0	-		
5	INO	M	550	4	10,11,11	2.05	4 (40%)	10,15,15	0.96	0
3	CYN	P	575	4	1,1,1	0.60	0	-		
5	INO	O	550	4	10,11,11	1.92	5 (50%)	10,15,15	1.39	2 (20%)
5	INO	N	550	4	10,11,11	1.94	4 (40%)	10,15,15	1.53	2 (20%)
5	INO	P	550	4	10,11,11	1.72	4 (40%)	10,15,15	1.21	2 (20%)
3	CYN	R	575	4	1,1,1	0.37	0	-		
3	CYN	Q	575	4	1,1,1	0.46	0	-		
5	INO	R	550	4	10,11,11	1.68	4 (40%)	10,15,15	1.24	2 (20%)
3	CYN	O	575	4	1,1,1	0.29	0	-		
5	INO	Q	550	4	10,11,11	1.68	3 (30%)	10,15,15	1.40	2 (20%)

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
5	INO	O	550	4	-	0/4/4/4	0/1/1/1
5	INO	M	550	4	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	INO	N	550	4	-	0/4/4/4	0/1/1/1
5	INO	P	550	4	-	0/4/4/4	0/1/1/1
5	INO	R	550	4	-	0/4/4/4	0/1/1/1
5	INO	Q	550	4	-	0/4/4/4	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	INO	O4-N1	-3.84	1.29	1.37
5	O	550	INO	O4-N1	-3.51	1.30	1.37
5	M	550	INO	O3-C2	-3.32	1.23	1.32
5	M	550	INO	O4-N1	-3.13	1.31	1.37
5	M	550	INO	C4-C7	2.86	1.55	1.49

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	550	INO	O2-C7-O1	-3.11	116.67	123.35
5	Q	550	INO	O2-C7-O1	-3.06	116.77	123.35
5	N	550	INO	O2-C7-C4	2.80	122.01	114.84
5	O	550	INO	O2-C7-O1	-2.79	117.36	123.35
5	R	550	INO	O2-C7-O1	-2.72	117.50	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	550	INO	1	0
3	P	575	CYN	1	0
3	R	575	CYN	2	0
3	Q	575	CYN	2	0
3	O	575	CYN	1	0
5	Q	550	INO	2	0

5.7 Other polymers [i](#)

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 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.