



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 05:37 am BST

PDB ID : 3PCL
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

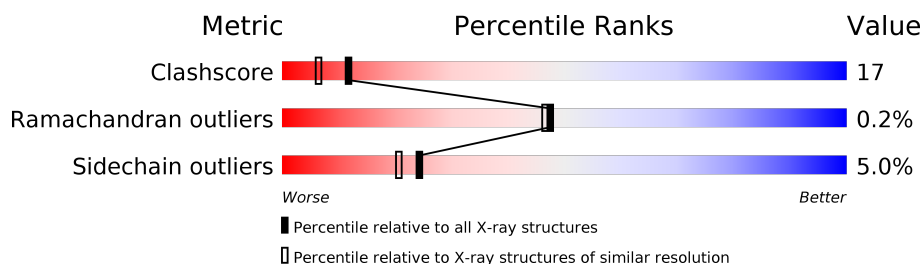
1 Overall quality at a glance

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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (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 on 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	69% 26% 5%
1	B	200	69% 26% . .
1	C	200	65% 32% .
1	D	200	69% 27% 5% .
1	E	200	62% 32% 5% .
1	F	200	58% 36% 6% .
2	M	238	66% 28% . .
2	N	238	66% 26% 5% .

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Mol	Chain	Length	Quality of chain
2	O	238	
2	P	238	
2	Q	238	
2	R	238	

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.

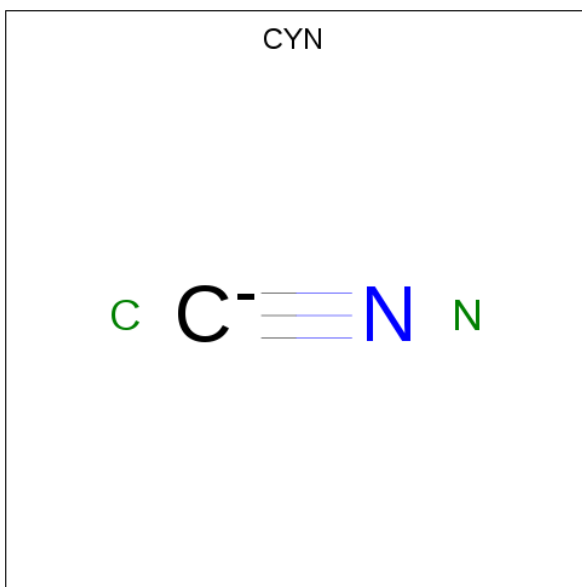
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

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

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

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).

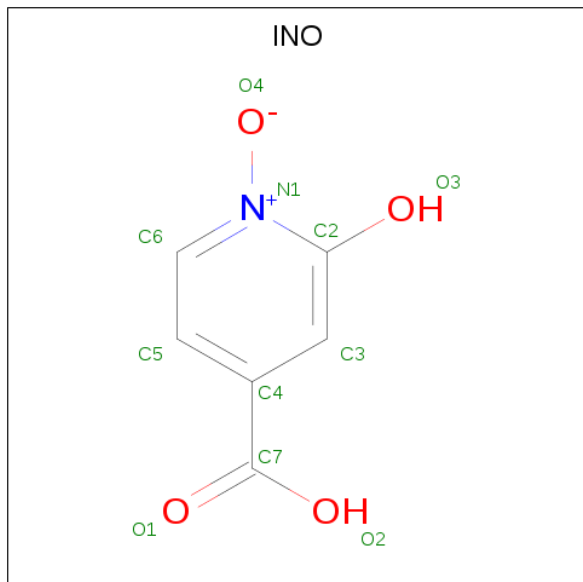


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	N	0	0
			2	1	1		
3	N	1	Total	C	N	0	0
			2	1	1		
3	O	1	Total	C	N	0	0
			2	1	1		
3	P	1	Total	C	N	0	0
			2	1	1		
3	Q	1	Total	C	N	0	0
			2	1	1		
3	R	1	Total	C	N	0	0
			2	1	1		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is 2-HYDROXYISONICOTINIC ACID N-OXIDE (three-letter code: INO) (formula: C₆H₅NO₄).



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

- Molecule 6 is water.

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

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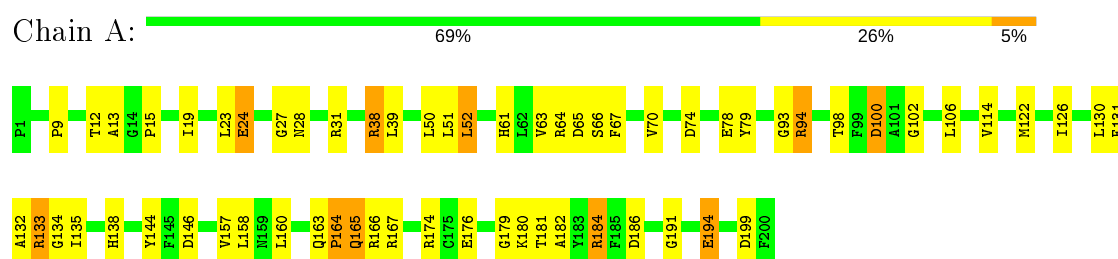
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	79	Total 79	O 79	0	0
6	O	157	Total 157	O 157	0	0
6	D	78	Total 78	O 78	0	0
6	P	152	Total 152	O 152	0	0
6	E	76	Total 76	O 76	0	0
6	Q	165	Total 165	O 165	0	0
6	F	82	Total 82	O 82	0	0
6	R	152	Total 152	O 152	0	0

3 Residue-property plots [i](#)

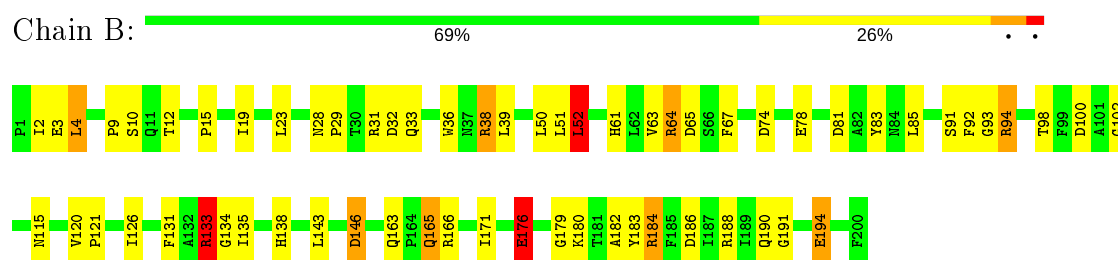
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

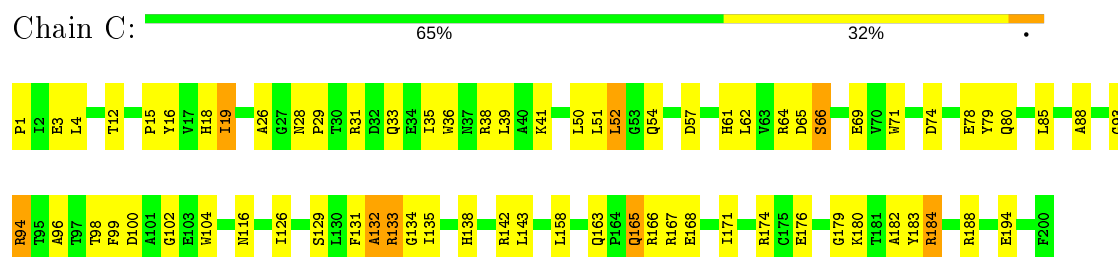
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



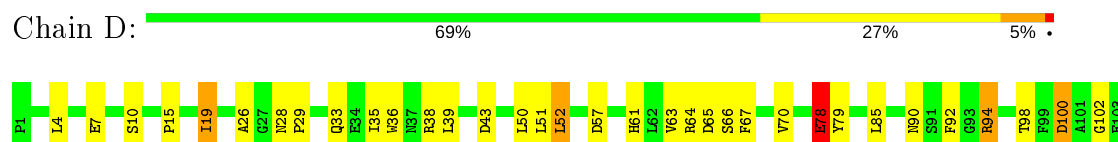
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



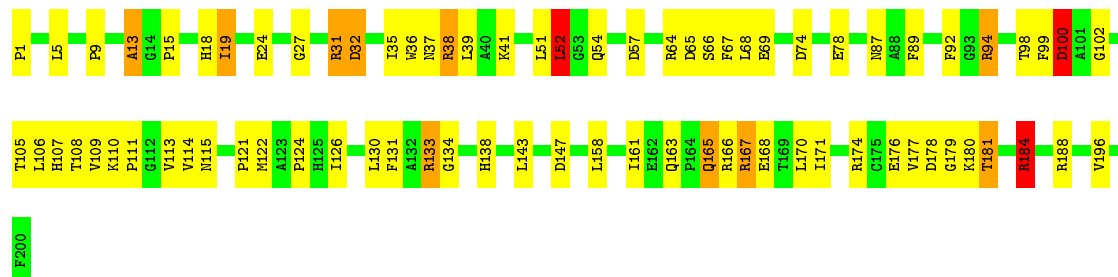
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE





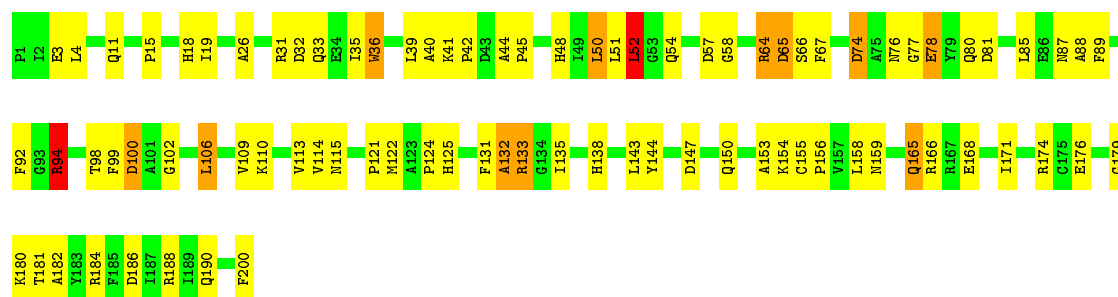
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 62% 32% 5%



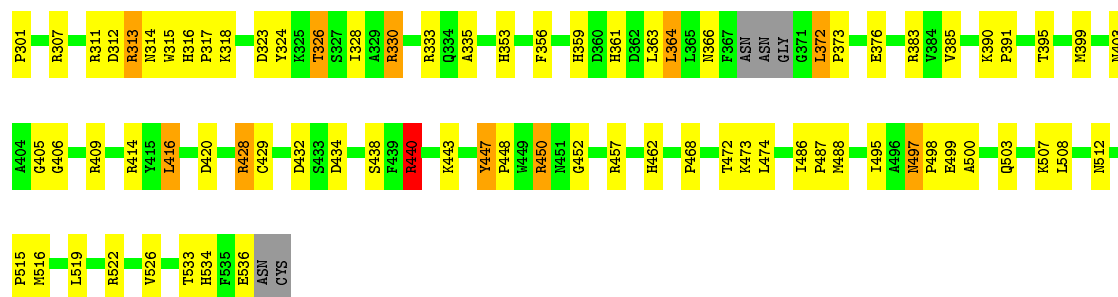
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 58% 36% 6%



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

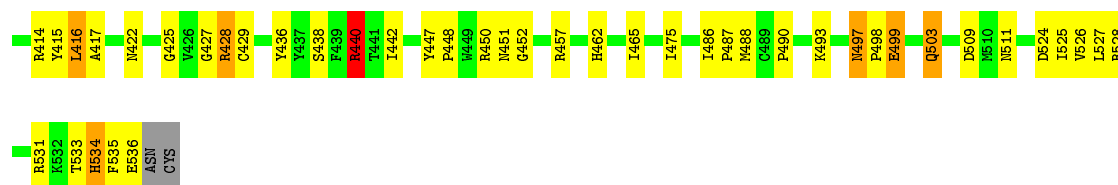
Chain M: 66% 28% 5%



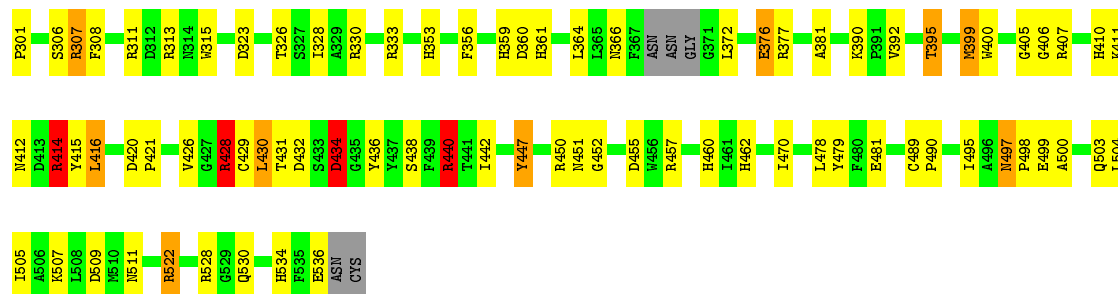
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N: 66% 26% 5%

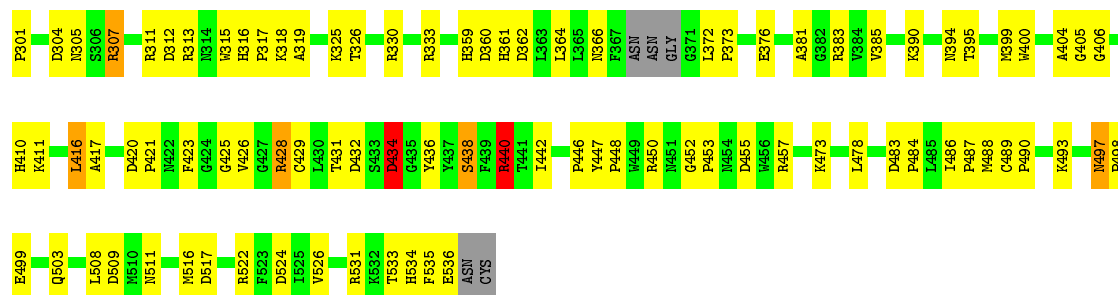




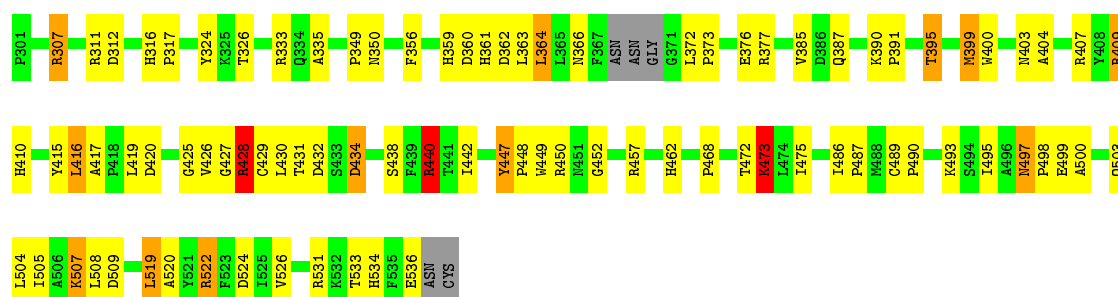
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

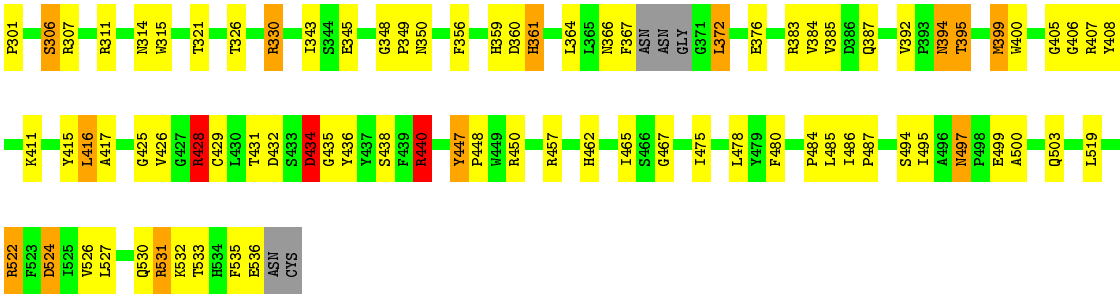


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





4 Data and refinement statistics

Xtriage (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	195.70 Å 128.00 Å 134.20 Å 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.	Xtriage
Total number of atoms	21960	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: INO, CYN, 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	1.01	2/1611 (0.1%)	1.73	25/2195 (1.1%)
1	B	1.05	2/1611 (0.1%)	1.81	33/2195 (1.5%)
1	C	1.01	1/1611 (0.1%)	1.58	22/2195 (1.0%)
1	D	1.02	1/1611 (0.1%)	1.66	24/2195 (1.1%)
1	E	1.00	0/1611	1.60	25/2195 (1.1%)
1	F	1.07	0/1611	1.66	25/2195 (1.1%)
2	M	1.10	0/1895	1.62	24/2580 (0.9%)
2	N	1.10	1/1895 (0.1%)	1.69	33/2580 (1.3%)
2	O	1.16	3/1895 (0.2%)	1.71	38/2580 (1.5%)
2	P	1.13	2/1895 (0.1%)	1.74	33/2580 (1.3%)
2	Q	1.15	1/1895 (0.1%)	1.77	33/2580 (1.3%)
2	R	1.13	1/1895 (0.1%)	1.69	27/2580 (1.0%)
All	All	1.08	14/21036 (0.1%)	1.69	342/28650 (1.2%)

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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	313	ARG	NE-CZ	7.55	1.42	1.33
2	Q	428	ARG	CD-NE	-6.72	1.35	1.46
2	O	428	ARG	CD-NE	-6.05	1.36	1.46
1	D	10	SER	CA-CB	5.77	1.61	1.52
2	P	440	ARG	CD-NE	-5.76	1.36	1.46

The worst 5 of 342 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	440	ARG	NE-CZ-NH2	-21.65	109.48	120.30
1	B	133	ARG	NE-CZ-NH1	21.22	130.91	120.30
2	N	440	ARG	NE-CZ-NH2	-19.64	110.48	120.30
1	A	94	ARG	NE-CZ-NH1	18.80	129.70	120.30
2	Q	428	ARG	CD-NE-CZ	18.64	149.70	123.60

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

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	48	0
1	B	1571	0	1499	52	0
1	C	1571	0	1499	57	0
1	D	1571	0	1499	55	0
1	E	1571	0	1499	70	0
1	F	1571	0	1499	86	0
2	M	1840	0	1794	67	0
2	N	1840	0	1794	57	0
2	O	1840	0	1794	62	0
2	P	1840	0	1794	77	0
2	Q	1840	0	1794	75	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	6	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	702	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 17.

The worst 5 of 702 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	1.10
1:B:165:GLN:NE2	1:B:165:GLN:H	1.52	1.06
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.44	0.99
1:E:165:GLN:H	1:E:165:GLN:HE21	1.02	0.97
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.45	0.95

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%)	29	22
1	D	198/200 (99%)	188 (95%)	9 (4%)	1 (0%)	29	22
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	29	22
2	M	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
2	N	229/238 (96%)	222 (97%)	6 (3%)	1 (0%)	34	29
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	34	29
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	10 (4%)	1 (0%)	34	29
All	All	2562/2628 (98%)	2445 (95%)	111 (4%)	6 (0%)	47	46

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%)	154 (95%)	8 (5%)	25	21
1	B	162/163 (99%)	153 (94%)	9 (6%)	21	16
1	C	162/163 (99%)	155 (96%)	7 (4%)	29	27
1	D	162/163 (99%)	153 (94%)	9 (6%)	21	16
1	E	162/163 (99%)	157 (97%)	5 (3%)	40	39
1	F	162/163 (99%)	155 (96%)	7 (4%)	29	27
2	M	196/202 (97%)	188 (96%)	8 (4%)	30	29
2	N	196/202 (97%)	189 (96%)	7 (4%)	35	33
2	O	196/202 (97%)	183 (93%)	13 (7%)	16	11
2	P	196/202 (97%)	187 (95%)	9 (5%)	27	23
2	Q	196/202 (97%)	184 (94%)	12 (6%)	18	14
2	R	196/202 (97%)	183 (93%)	13 (7%)	16	11
All	All	2148/2190 (98%)	2041 (95%)	107 (5%)	24	21

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	440	ARG
1	D	165	GLN
2	R	395	THR
2	O	497	ASN
1	D	43	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	497	ASN
2	P	361	HIS
2	R	497	ASN
2	O	503	GLN
2	O	530	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 carbohydrates 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	$\# Z > 2$
5	INO	P	550	4	6,11,11	3.34	2 (33%)	7,15,15	0.61	0
5	INO	Q	550	4	6,11,11	3.21	2 (33%)	7,15,15	0.75	0
5	INO	R	550	4	6,11,11	3.03	2 (33%)	7,15,15	0.67	0
3	CYN	Q	575	4	0,1,1	0.00	-	-		
3	CYN	R	575	4	0,1,1	0.00	-	-		
5	INO	N	550	4	6,11,11	2.88	2 (33%)	7,15,15	0.98	0
3	CYN	P	575	4	0,1,1	0.00	-	-		
5	INO	O	550	4	6,11,11	3.21	2 (33%)	7,15,15	1.02	0
3	CYN	M	575	4	0,1,1	0.00	-	-		
5	INO	M	550	4	6,11,11	3.68	2 (33%)	7,15,15	0.93	0
3	CYN	N	575	4	0,1,1	0.00	-	-		
3	CYN	O	575	4	0,1,1	0.00	-	-		

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	P	550	4	-	0/0/4/4	0/1/1/1
5	INO	Q	550	4	-	0/0/4/4	0/1/1/1

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	550	INO	C4-C7	8.29	1.55	1.47
5	P	550	INO	C4-C7	7.56	1.54	1.47
5	Q	550	INO	C4-C7	7.28	1.54	1.47
5	O	550	INO	C4-C7	7.18	1.54	1.47
5	R	550	INO	C4-C7	6.85	1.54	1.47

There are no bond angle outliers.

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	Q	550	INO	2	0
3	Q	575	CYN	2	0
3	R	575	CYN	2	0
3	P	575	CYN	1	0
5	M	550	INO	1	0
3	O	575	CYN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.