



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:07 AM GMT

PDB ID : 3PCL  
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-  
PLEXED WITH 2-HYDROXYISONICOTINICACID 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 validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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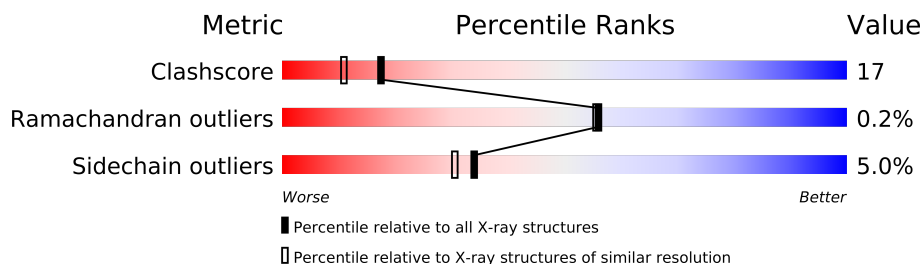
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	
1	B	200	
1	C	200	
1	D	200	
1	E	200	
1	F	200	
2	M	238	
2	N	238	
2	O	238	
2	P	238	
2	Q	238	
2	R	238	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21960 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

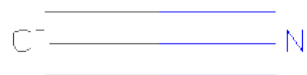
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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).

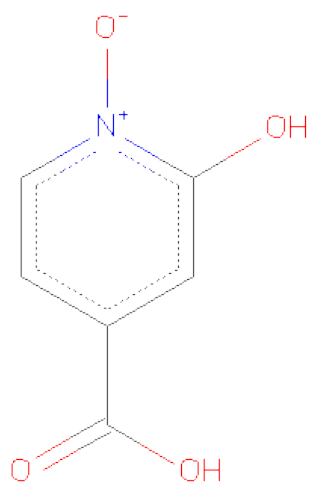


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	N	0	0
			2	1	1		
3	N	1	Total	C	N	0	0
			2	1	1		
3	O	1	Total	C	N	0	0
			2	1	1		
3	P	1	Total	C	N	0	0
			2	1	1		
3	Q	1	Total	C	N	0	0
			2	1	1		
3	R	1	Total	C	N	0	0
			2	1	1		

- 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-HYDROXYISONICOTINICACID N-OXIDE (three-letter code: INO) (formula:  $C_6H_5NO_4$ ).



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	B	78	Total	O	0	0
			78	78		
6	C	79	Total	O	0	0
			79	79		
6	D	78	Total	O	0	0
			78	78		

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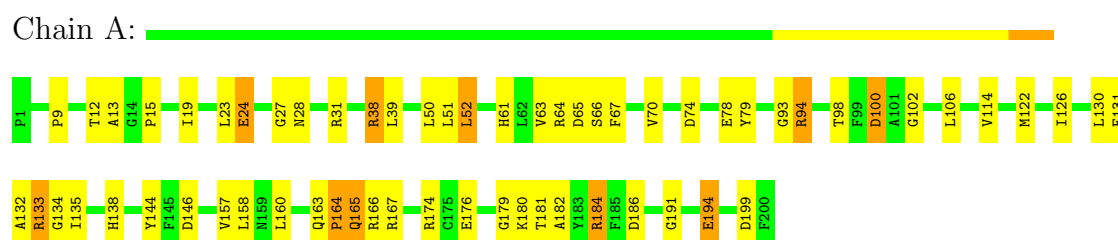
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	76	Total 76	O 76	0	0
6	F	82	Total 82	O 82	0	0
6	M	156	Total 156	O 156	0	0
6	N	159	Total 159	O 159	0	0
6	O	157	Total 157	O 157	0	0
6	P	152	Total 152	O 152	0	0
6	Q	165	Total 165	O 165	0	0
6	R	152	Total 152	O 152	0	0

### 3 Residue-property plots

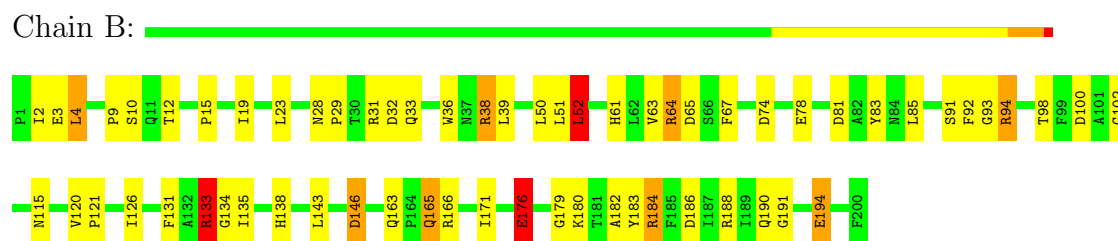
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

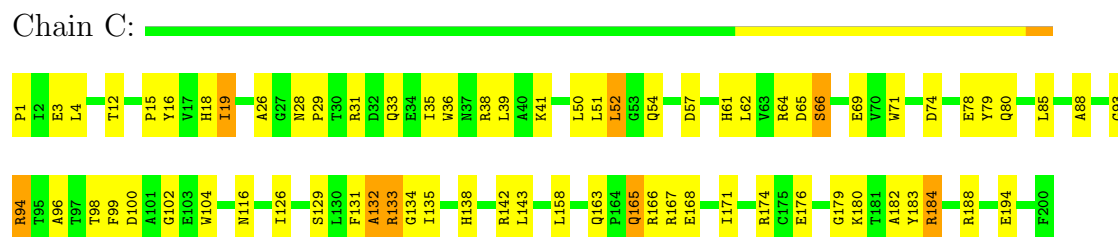
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



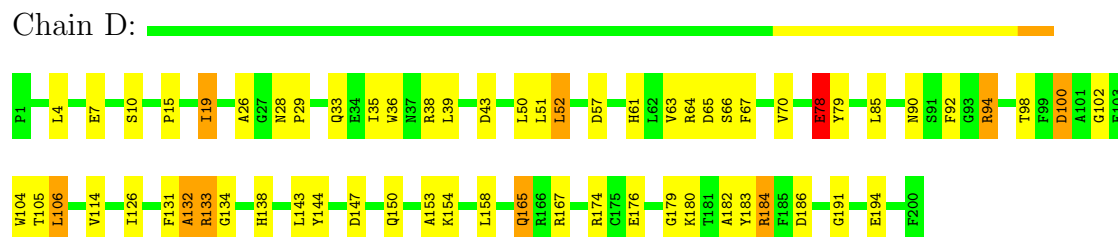
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

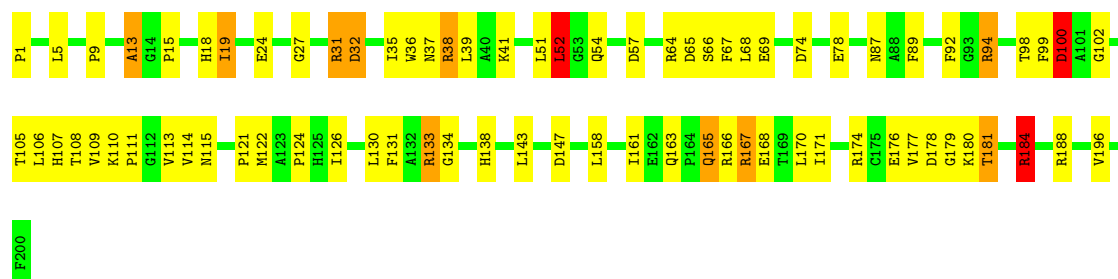


#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



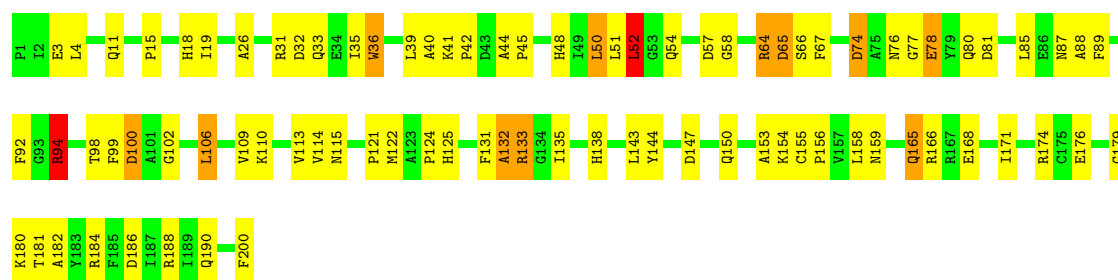
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

## Chain E:



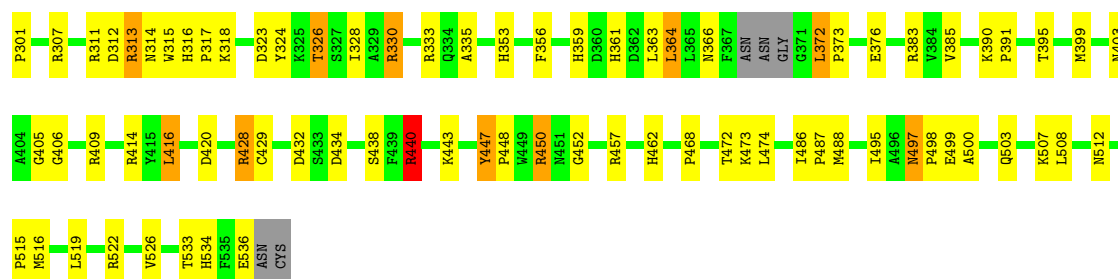
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

## Chain F:



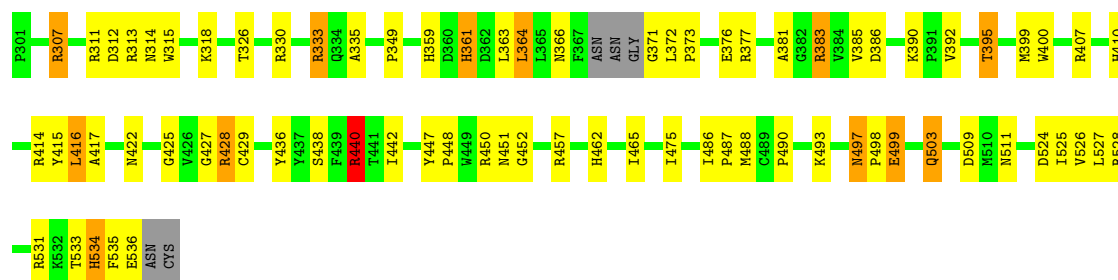
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

## Chain M:



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

## Chain N:



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

## Chain O:







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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.	Xtriage
Total number of atoms	21960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	1	0	0	0	0
4	N	1	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

The worst 5 of 702 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 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	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%)	38	31
1	D	198/200 (99%)	188 (95%)	9 (4%)	1 (0%)	38	31
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	38	31
2	M	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
2	N	229/238 (96%)	222 (97%)	6 (3%)	1 (0%)	43	39
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	43	39
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	10 (4%)	1 (0%)	43	39
All	All	2562/2628 (98%)	2445 (95%)	111 (4%)	6 (0%)	56	55

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 ⓘ

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%)	35	31
1	B	162/163 (99%)	153 (94%)	9 (6%)	30	25
1	C	162/163 (99%)	155 (96%)	7 (4%)	40	38
1	D	162/163 (99%)	153 (94%)	9 (6%)	30	25
1	E	162/163 (99%)	157 (97%)	5 (3%)	52	54
1	F	162/163 (99%)	155 (96%)	7 (4%)	40	38
2	M	196/202 (97%)	188 (96%)	8 (4%)	41	40
2	N	196/202 (97%)	189 (96%)	7 (4%)	47	47
2	O	196/202 (97%)	183 (93%)	13 (7%)	24	17
2	P	196/202 (97%)	187 (95%)	9 (5%)	37	34
2	Q	196/202 (97%)	184 (94%)	12 (6%)	26	21
2	R	196/202 (97%)	183 (93%)	13 (7%)	24	17
All	All	2148/2190 (98%)	2041 (95%)	107 (5%)	34	30

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 chains 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 ⓘ

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	M	550	4	11,11,11	1.68	4 (36%)	15,15,15	0.96	0
3	CYN	M	575	4	1,1,1	0.67	0	0,0,0	0.00	-
5	INO	N	550	4	11,11,11	1.42	2 (18%)	15,15,15	1.24	2 (13%)
3	CYN	N	575	4	1,1,1	0.64	0	0,0,0	0.00	-
5	INO	O	550	4	11,11,11	1.57	3 (27%)	15,15,15	1.35	3 (20%)
3	CYN	O	575	4	1,1,1	0.47	0	0,0,0	0.00	-
5	INO	P	550	4	11,11,11	1.67	4 (36%)	15,15,15	1.17	2 (13%)
3	CYN	P	575	4	1,1,1	0.86	0	0,0,0	0.00	-
5	INO	Q	550	4	11,11,11	1.30	1 (9%)	15,15,15	1.16	2 (13%)
3	CYN	Q	575	4	1,1,1	0.68	0	0,0,0	0.00	-
5	INO	R	550	4	11,11,11	1.36	1 (9%)	15,15,15	1.26	3 (20%)
3	CYN	R	575	4	1,1,1	0.58	0	0,0,0	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	M	550	4	-	0/4/4/4	0/1/1/1
3	CYN	M	575	4	-	0/0/0/0	0/0/0/0

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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
3	CYN	N	575	4	-	0/0/0/0	0/0/0/0
5	INO	O	550	4	-	0/4/4/4	0/1/1/1
3	CYN	O	575	4	-	0/0/0/0	0/0/0/0
5	INO	P	550	4	-	0/4/4/4	0/1/1/1
3	CYN	P	575	4	-	0/0/0/0	0/0/0/0
5	INO	Q	550	4	-	0/4/4/4	0/1/1/1
3	CYN	Q	575	4	-	0/0/0/0	0/0/0/0
5	INO	R	550	4	-	0/4/4/4	0/1/1/1
3	CYN	R	575	4	-	0/0/0/0	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	550	INO	C4-C7	3.07	1.55	1.49
5	P	550	INO	C6-N1	-2.73	1.32	1.36
5	P	550	INO	C4-C7	2.72	1.54	1.49
5	Q	550	INO	C4-C7	2.58	1.54	1.49
5	O	550	INO	C6-N1	-2.54	1.32	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	550	INO	O2-C7-O1	-2.93	116.70	123.35
5	Q	550	INO	O2-C7-O1	-2.88	116.82	123.35
5	O	550	INO	O2-C7-O1	-2.64	117.35	123.35
5	N	550	INO	O2-C7-C4	2.63	121.96	115.01
5	R	550	INO	O2-C7-O1	-2.57	117.51	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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.