wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2026 – 05:32 AM UTC

PDB ID	:	3PCM / pdb_00003pcm
Title	:	STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COMPLEXED WITH 6-HYDROXYNICOTINIC ACID N-OXIDE AND CYANIDE
Authors	:	Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1997-07-18
Resolution	:	2.25 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 (i) 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 (i)) were used in the production of this report:

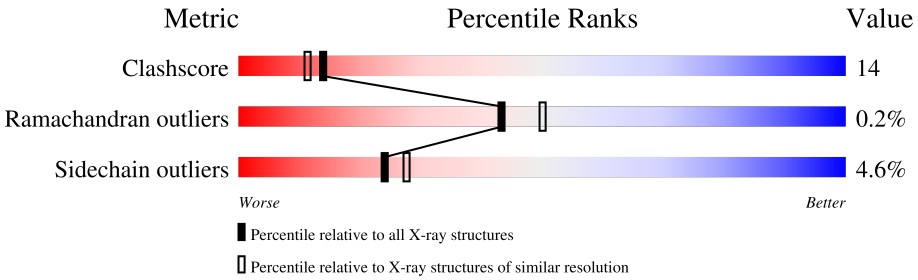
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	68% 27% .
1	B	200	73% 22% 5%
1	C	200	69% 27% .
1	D	200	66% 28% 6%
1	E	200	68% 29% .
1	F	200	61% 34% 5%
2	M	238	65% 29% . .
2	N	238	71% 22% 5% .

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

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21966 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.

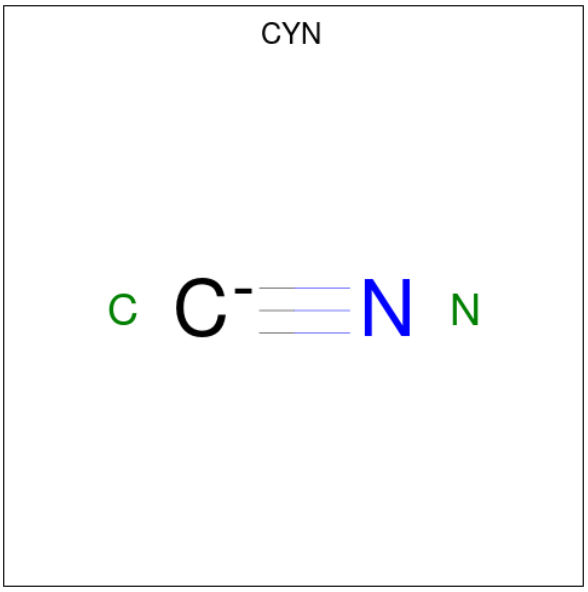
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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 (CCD ID: CYN) (formula: CN).

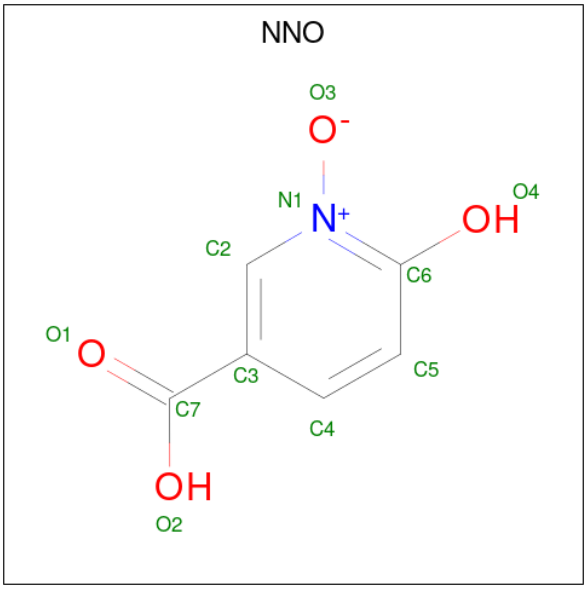


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C N 2 1 1	0	0
3	N	1	Total C N 2 1 1	0	0
3	O	1	Total C N 2 1 1	0	0
3	P	1	Total C N 2 1 1	0	0
3	Q	1	Total C N 2 1 1	0	0
3	R	1	Total C N 2 1 1	0	0

- 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 6-HYDROXYISONICOTINIC ACID N-OXIDE (CCD ID: NNO) (formula: $C_6H_5NO_4$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	77	Total O 77 77	0	0
6	M	154	Total O 154 154	0	0
6	B	86	Total O 86 86	0	0
6	N	156	Total O 156 156	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	78	Total O 78 78	0	0
6	O	156	Total O 156 156	0	0
6	D	80	Total O 80 80	0	0
6	P	151	Total O 151 151	0	0
6	E	79	Total O 79 79	0	0
6	Q	161	Total O 161 161	0	0
6	F	78	Total O 78 78	0	0
6	R	160	Total O 160 160	0	0

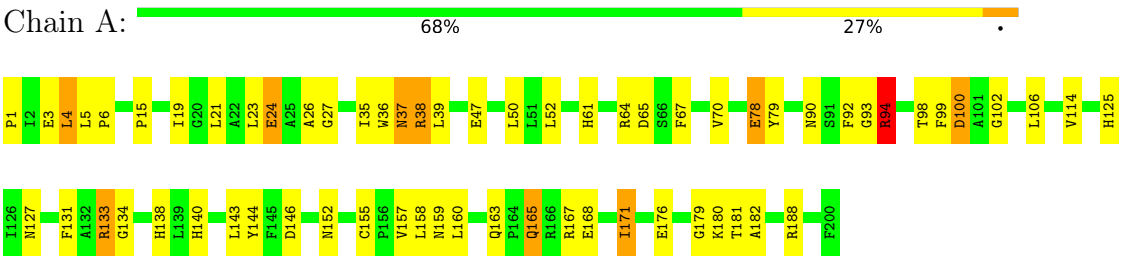
3 Residue-property plots (i)

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.

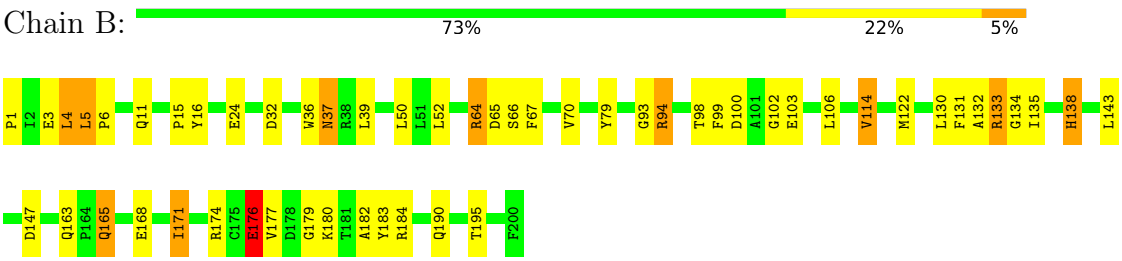
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A:



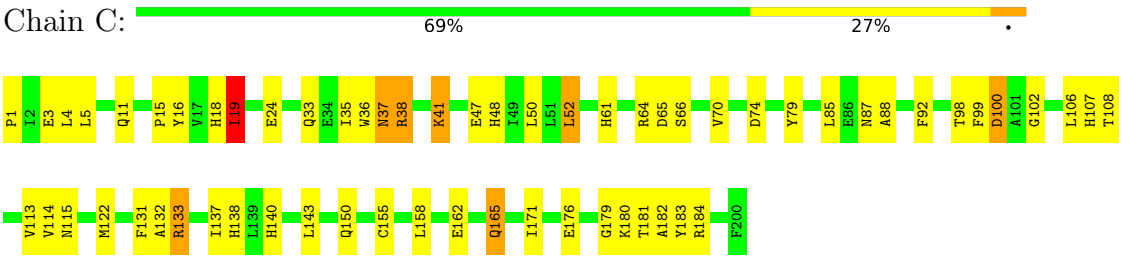
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B:



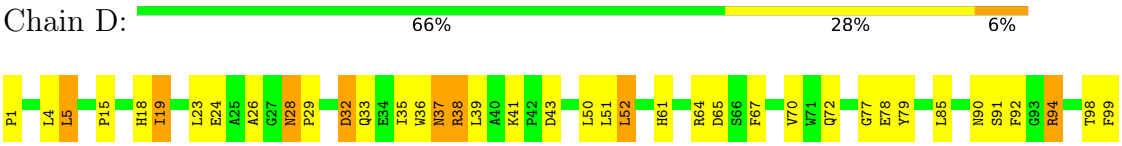
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

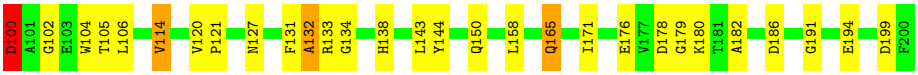
Chain C:



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

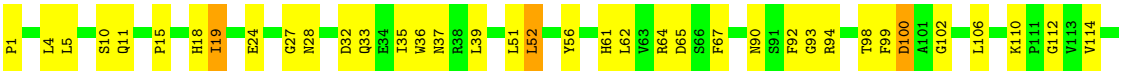
Chain D:

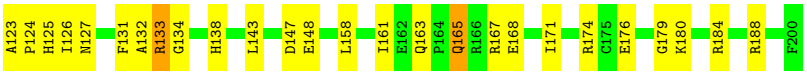




• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

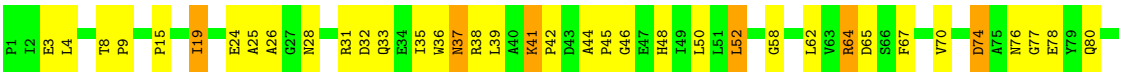
Chain E:





• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:

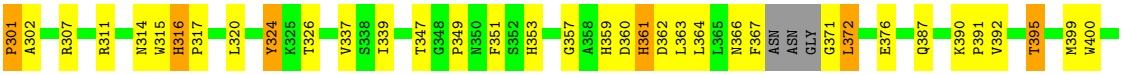


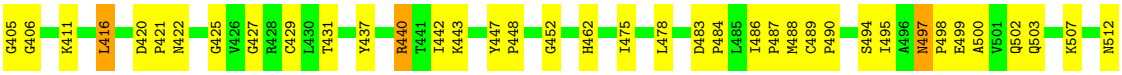




• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:

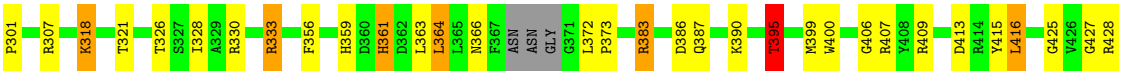


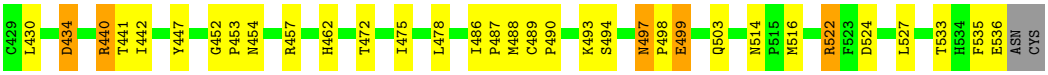




• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

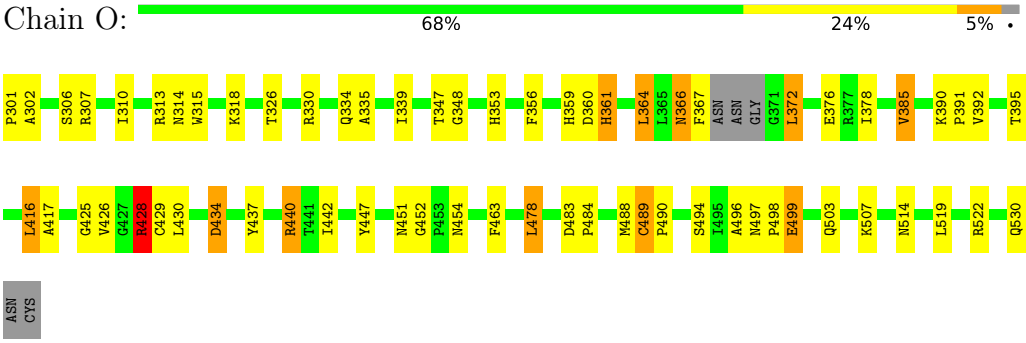
Chain N:





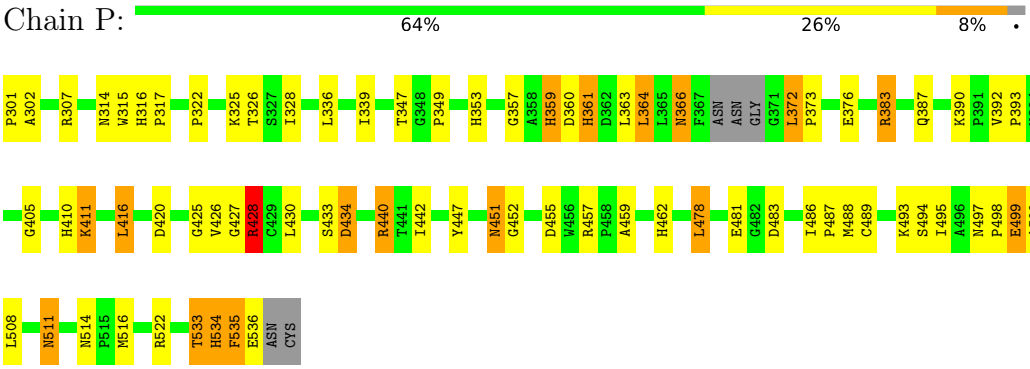
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:



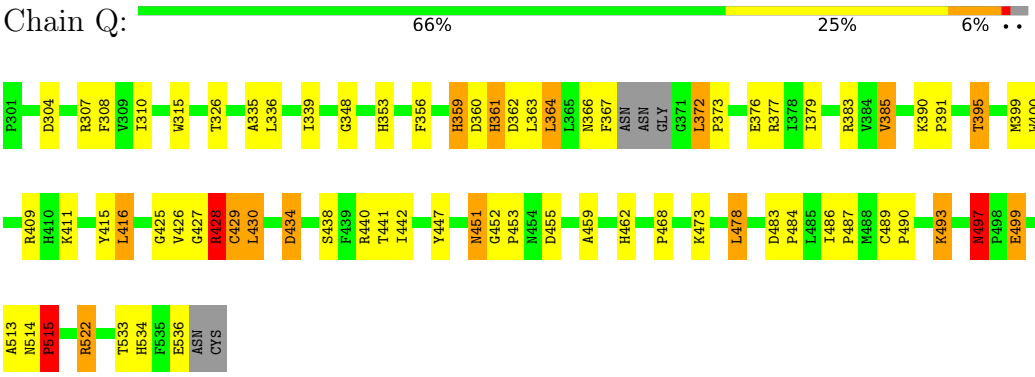
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



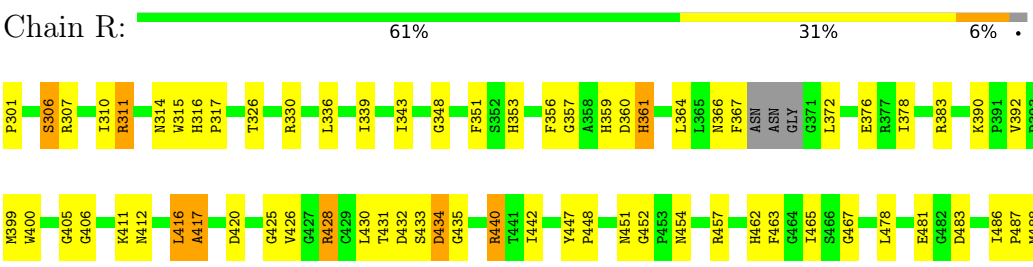
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

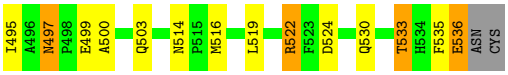
Chain Q:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:




I495
A496
N497
P498
E499
A500
Q503
N514
P515
M516
L519
R522
F523
D524
Q530
T533
H534
F535
E536
ASN
CYS

4 Data and refinement statistics (i)

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	196.10Å 127.30Å 134.50Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.25	Depositor
% Data completeness (in resolution range)	91.0 (6.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21966	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: NNO, FE, CYN

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	1.11	1/1611 (0.1%)	1.73	20/2195 (0.9%)
1	B	1.11	1/1611 (0.1%)	1.70	17/2195 (0.8%)
1	C	1.12	1/1611 (0.1%)	1.68	19/2195 (0.9%)
1	D	1.10	0/1611	1.67	15/2195 (0.7%)
1	E	1.13	0/1611	1.62	10/2195 (0.5%)
1	F	1.20	1/1611 (0.1%)	1.75	20/2195 (0.9%)
2	M	1.19	0/1895	1.73	23/2580 (0.9%)
2	N	1.19	3/1895 (0.2%)	1.71	20/2580 (0.8%)
2	O	1.19	1/1895 (0.1%)	1.80	36/2580 (1.4%)
2	P	1.25	1/1895 (0.1%)	1.76	38/2580 (1.5%)
2	Q	1.28	4/1895 (0.2%)	1.79	34/2580 (1.3%)
2	R	1.25	2/1895 (0.1%)	1.78	35/2580 (1.4%)
All	All	1.18	15/21036 (0.1%)	1.73	287/28650 (1.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	451	ASN	CA-C	9.36	1.56	1.52
2	P	451	ASN	CA-C	9.11	1.56	1.52
2	Q	451	ASN	CA-C	8.41	1.56	1.52
1	A	94	ARG	CD-NE	-6.88	1.36	1.46
2	Q	428	ARG	CD-NE	-6.10	1.37	1.46

The worst 5 of 287 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ARG	CD-NE-CZ	19.04	151.05	124.40
2	Q	428	ARG	CD-NE-CZ	12.42	141.79	124.40
2	O	451	ASN	O-C-N	10.95	128.93	120.83
2	O	428	ARG	CD-NE-CZ	10.82	139.55	124.40
2	N	452	GLY	N-CA-C	-10.73	99.25	112.23

There are no chirality outliers.

There are no planarity outliers.

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	48	0
1	B	1571	0	1499	41	0
1	C	1571	0	1499	43	0
1	D	1571	0	1499	55	0
1	E	1571	0	1499	55	0
1	F	1571	0	1499	61	0
2	M	1840	0	1794	58	0
2	N	1840	0	1794	52	0
2	O	1840	0	1794	51	0
2	P	1840	0	1794	57	0
2	Q	1840	0	1794	60	0
2	R	1840	0	1794	61	0
3	M	2	0	0	1	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	1	0
3	R	2	0	0	1	0
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	0	0
5	R	11	0	3	0	0
6	A	77	0	0	1	0
6	B	86	0	0	0	0
6	C	78	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	80	0	0	1	0
6	E	79	0	0	3	0
6	F	78	0	0	0	0
6	M	154	0	0	7	0
6	N	156	0	0	4	0
6	O	156	0	0	4	0
6	P	151	0	0	7	0
6	Q	161	0	0	5	0
6	R	160	0	0	5	0
All	All	21966	0	19776	582	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 14.

The worst 5 of 582 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:165:GLN:H	1:B:165:GLN:NE2	1.49	1.09
1:C:64:ARG:NH1	1:C:100:ASP:O	1.92	1.02
1:F:64:ARG:NH1	1:F:100:ASP:O	1.92	1.00
1:B:165:GLN:HE21	1:B:165:GLN:N	1.59	1.00
1:D:64:ARG:NH1	1:D:100:ASP:O	1.93	1.00

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	178/200 (89%)	169 (95%)	9 (5%)	0	100	100
1	B	198/200 (99%)	191 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	D	198/200 (99%)	187 (94%)	10 (5%)	1 (0%)	24	24
1	E	198/200 (99%)	186 (94%)	12 (6%)	0	100	100
1	F	198/200 (99%)	187 (94%)	9 (4%)	2 (1%)	12	10
2	M	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	N	229/238 (96%)	219 (96%)	9 (4%)	1 (0%)	30	31
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	30	31
2	Q	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	R	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	30	31
All	All	2542/2628 (97%)	2431 (96%)	105 (4%)	6 (0%)	43	50

5 of 6 Ramachandran outliers are listed below:

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

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	20
1	B	162/163 (99%)	155 (96%)	7 (4%)	26	31
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	31
1	D	162/163 (99%)	154 (95%)	8 (5%)	22	24
1	E	162/163 (99%)	156 (96%)	6 (4%)	30	37
1	F	162/163 (99%)	156 (96%)	6 (4%)	30	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	196/202 (97%)	187 (95%)	9 (5%)	24 28
2	N	196/202 (97%)	191 (97%)	5 (3%)	40 50
2	O	196/202 (97%)	186 (95%)	10 (5%)	21 23
2	P	196/202 (97%)	186 (95%)	10 (5%)	21 23
2	Q	196/202 (97%)	184 (94%)	12 (6%)	17 17
2	R	196/202 (97%)	187 (95%)	9 (5%)	24 28
All	All	2148/2190 (98%)	2050 (95%)	98 (5%)	24 28

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	416	LEU
2	Q	364	LEU
2	P	433	SER
1	E	4	LEU
2	Q	429	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	502	GLN
2	Q	422	ASN
2	R	530	GLN
2	P	503	GLN
1	E	165	GLN

5.3.3 RNA (i)

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	P	575	4	1,1,1	0.52	0	-		
3	CYN	Q	575	4	1,1,1	0.50	0	-		
5	NNO	O	550	4	11,11,11	2.17	3 (27%)	11,15,15	1.67	2 (18%)
5	NNO	R	550	4	11,11,11	1.93	3 (27%)	11,15,15	1.49	2 (18%)
5	NNO	Q	550	4	11,11,11	2.04	2 (18%)	11,15,15	1.23	1 (9%)
3	CYN	M	575	4	1,1,1	0.62	0	-		
3	CYN	N	575	4	1,1,1	0.53	0	-		
3	CYN	R	575	4	1,1,1	0.55	0	-		
3	CYN	O	575	4	1,1,1	0.52	0	-		
5	NNO	P	550	4	11,11,11	1.93	4 (36%)	11,15,15	1.69	2 (18%)
5	NNO	N	550	4	11,11,11	2.19	4 (36%)	11,15,15	1.42	2 (18%)
5	NNO	M	550	4	11,11,11	2.04	2 (18%)	11,15,15	1.32	1 (9%)

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	NNO	O	550	4	-	0/4/4/4	0/1/1/1
5	NNO	R	550	4	-	0/4/4/4	0/1/1/1
5	NNO	Q	550	4	-	0/4/4/4	0/1/1/1
5	NNO	P	550	4	-	0/4/4/4	0/1/1/1
5	NNO	N	550	4	-	0/4/4/4	0/1/1/1
5	NNO	M	550	4	-	0/4/4/4	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	NNO	O3-N1	-5.62	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	550	NNO	O3-N1	-5.48	1.26	1.37
5	M	550	NNO	O3-N1	-5.17	1.27	1.37
5	O	550	NNO	O3-N1	-5.01	1.27	1.37
5	P	550	NNO	O3-N1	-4.62	1.28	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	550	NNO	O2-C7-C3	3.46	123.71	114.84
5	O	550	NNO	O2-C7-O1	-3.22	116.44	123.35
5	N	550	NNO	O2-C7-O1	-3.00	116.91	123.35
5	P	550	NNO	O2-C7-C3	2.92	122.34	114.84
5	P	550	NNO	O2-C7-O1	-2.88	117.17	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

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