



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:06 AM UTC

PDB ID : 3PCJ / pdb_00003pcj
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 2-HYDROXYISONICOTINIC ACID N-OXIDE
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-18
Resolution : 2.13 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

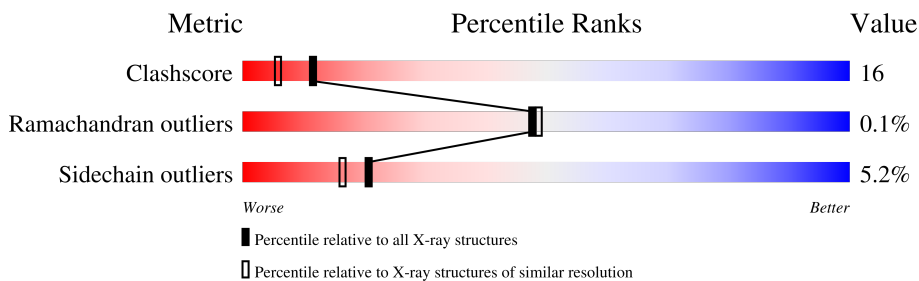
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)





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	
1	B	200	
1	C	200	
1	D	200	
1	E	200	
1	F	200	
2	M	238	
2	N	238	

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Mol	Chain	Length	Quality of chain
2	O	238	 59% 31% 8% •
2	P	238	 62% 29% 7% •
2	Q	238	 63% 29% 6% •
2	R	238	 56% 32% 9% ••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21978 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

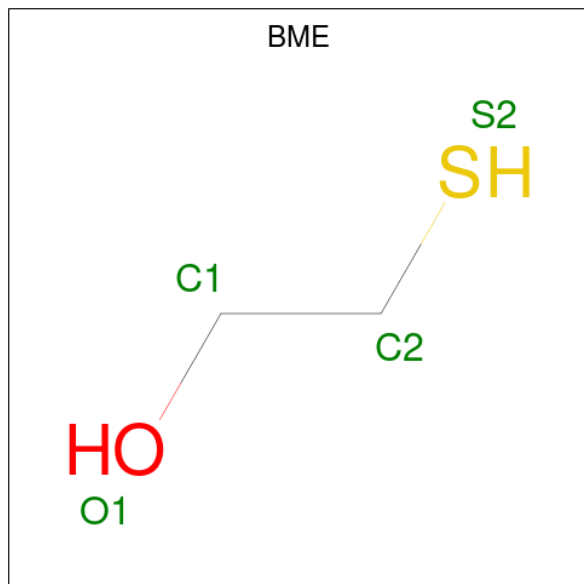
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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 FE (III) ION (CCD ID: FE) (formula: Fe).

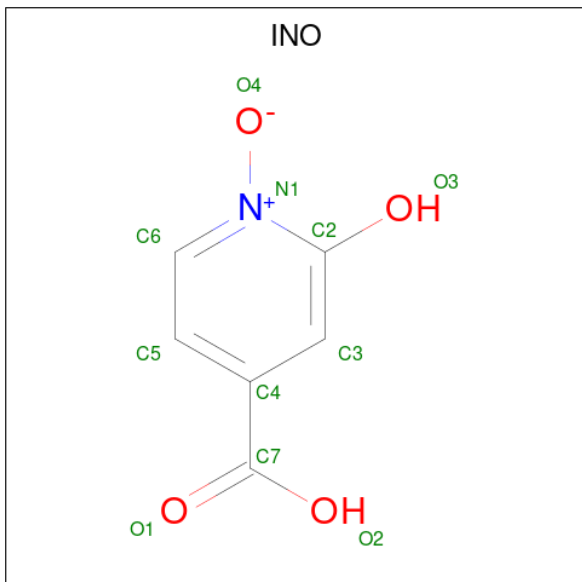
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O S 4 2 1 1	0	0
4	N	1	Total C O S 4 2 1 1	0	0
4	O	1	Total C O S 4 2 1 1	0	0
4	P	1	Total C O S 4 2 1 1	0	0
4	Q	1	Total C O S 4 2 1 1	0	0
4	R	1	Total C O S 4 2 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	79	79	79	0	0
6	M	155	155	155	0	0
6	B	78	78	78	0	0
6	N	163	163	163	0	0

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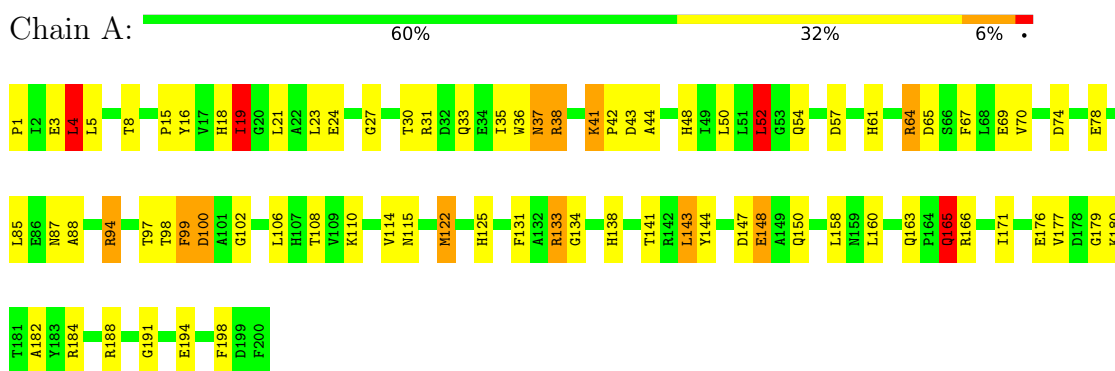
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	76	Total O 76 76	0	0
6	O	158	Total O 158 158	0	0
6	D	79	Total O 79 79	0	0
6	P	149	Total O 149 149	0	0
6	E	81	Total O 81 81	0	0
6	Q	160	Total O 160 160	0	0
6	F	75	Total O 75 75	0	0
6	R	163	Total O 163 163	0	0

3 Residue-property plots [i](#)

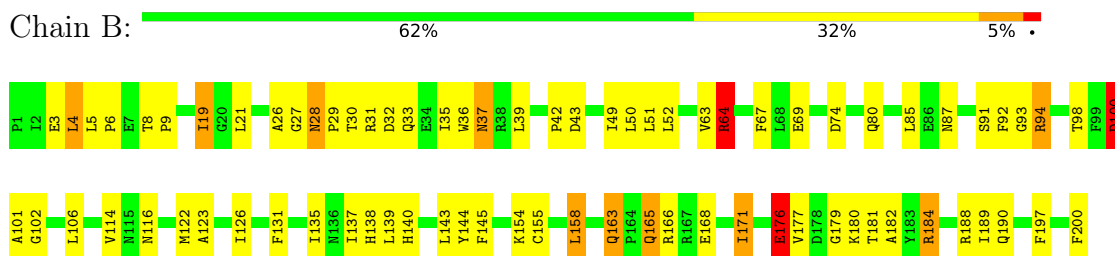
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

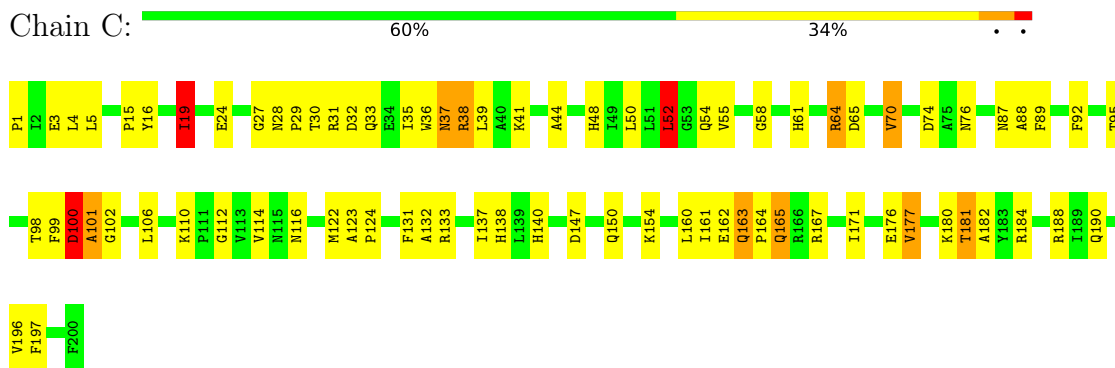
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



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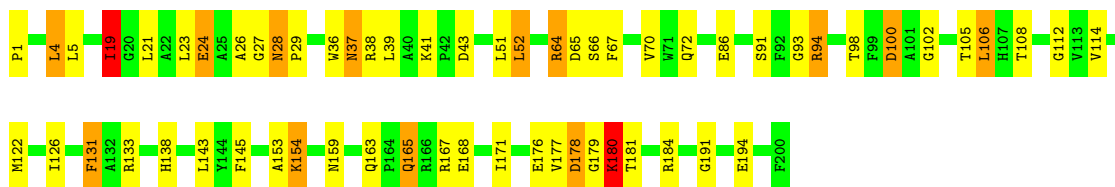


- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



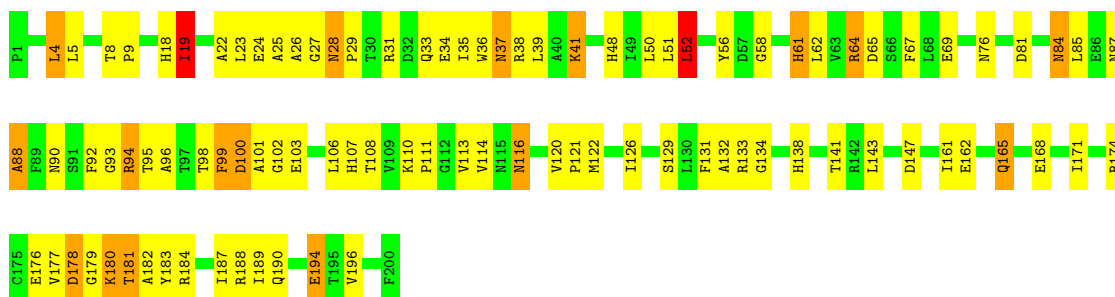
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D:  70% 23% 6% .



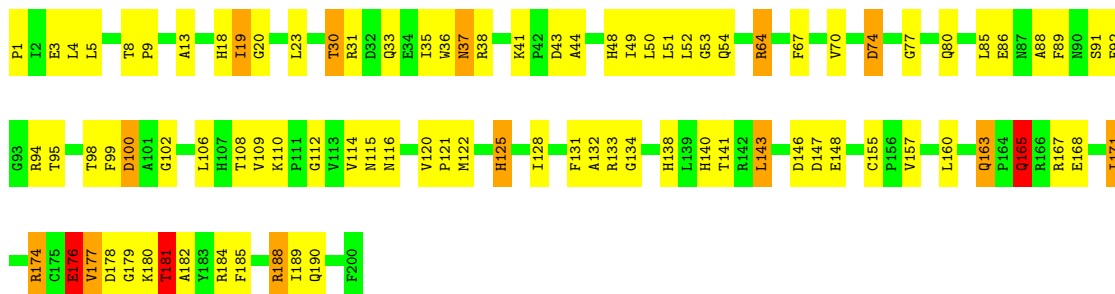
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:  52% 38% 8% .



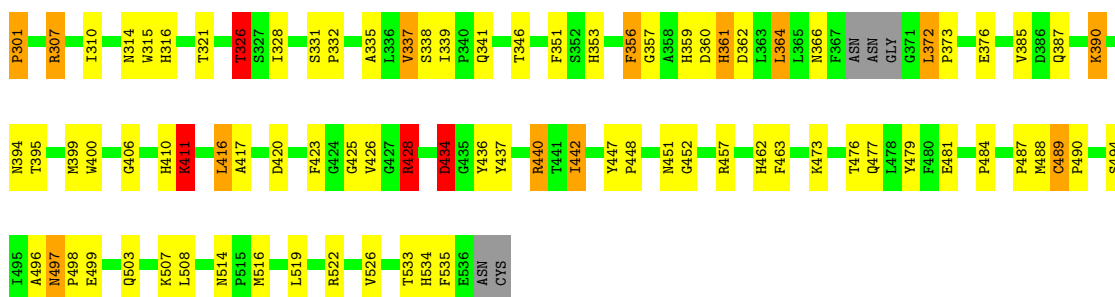
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:  54% 38% 6% .

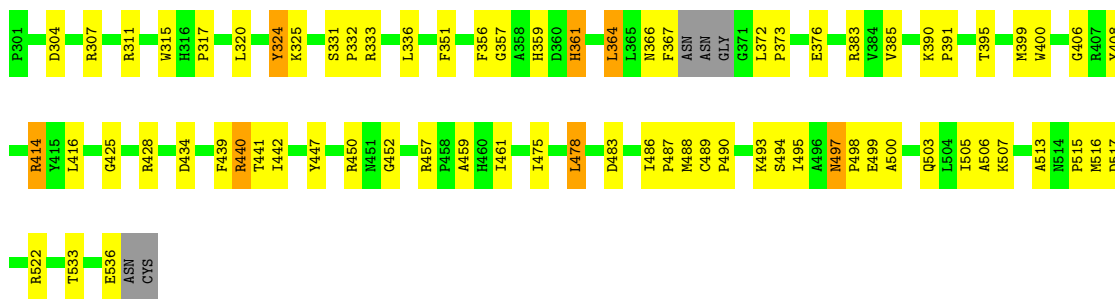


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

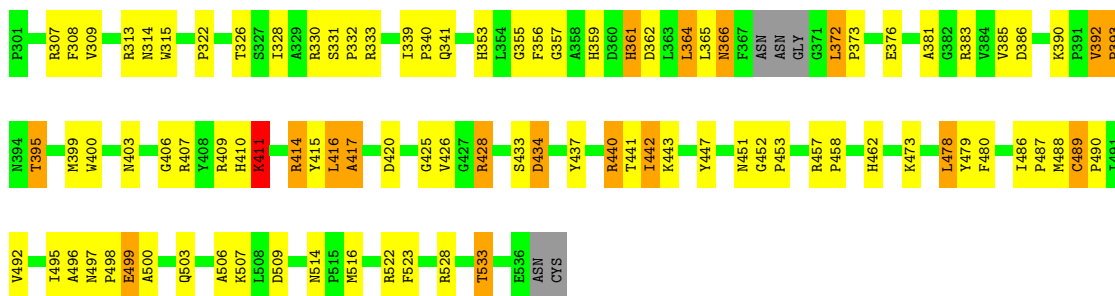
Chain M:  62% 29% 5% .



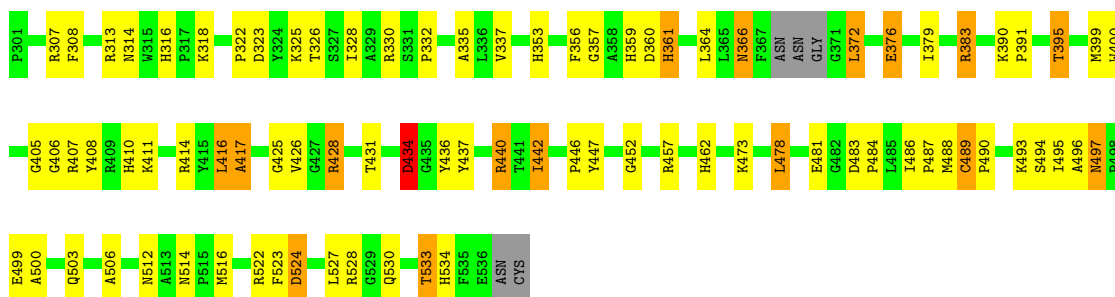
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



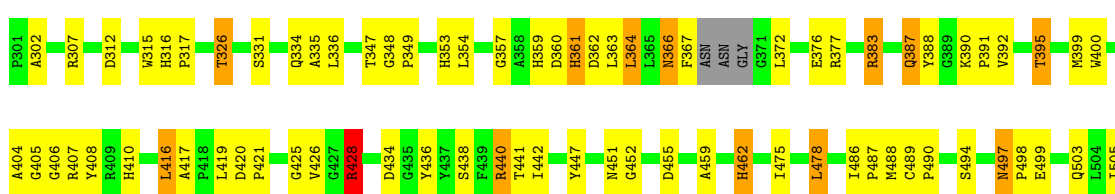
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

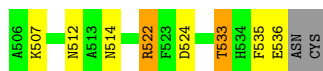


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



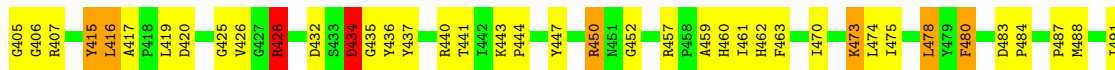
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





● Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 56% 32% 9% ..



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	196.20Å 127.10Å 133.70Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.13	Depositor
% Data completeness (in resolution range)	96.0 (6.00-2.13)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	21978	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: INO, BME, 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	1.27	4/1611 (0.2%)	1.91	37/2195 (1.7%)
1	B	1.25	2/1611 (0.1%)	1.89	36/2195 (1.6%)
1	C	1.28	1/1611 (0.1%)	1.86	30/2195 (1.4%)
1	D	1.28	1/1611 (0.1%)	1.77	27/2195 (1.2%)
1	E	1.32	3/1611 (0.2%)	1.87	32/2195 (1.5%)
1	F	1.39	6/1611 (0.4%)	1.91	35/2195 (1.6%)
2	M	1.33	1/1895 (0.1%)	1.93	37/2580 (1.4%)
2	N	1.34	5/1895 (0.3%)	1.85	28/2580 (1.1%)
2	O	1.37	3/1895 (0.2%)	1.92	54/2580 (2.1%)
2	P	1.35	4/1895 (0.2%)	1.87	40/2580 (1.6%)
2	Q	1.39	4/1895 (0.2%)	1.83	26/2580 (1.0%)
2	R	1.40	4/1895 (0.2%)	1.92	45/2580 (1.7%)
All	All	1.33	38/21036 (0.2%)	1.88	427/28650 (1.5%)

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	B	0	1
2	R	0	1
All	All	0	2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	451	ASN	CA-C	10.39	1.57	1.52
1	C	100	ASP	N-CA	7.67	1.51	1.46
1	A	94	ARG	CD-NE	-7.65	1.35	1.46
2	N	441	THR	CA-CB	7.15	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	128	ILE	CA-CB	6.17	1.63	1.54

The worst 5 of 427 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	133	ARG	CD-NE-CZ	17.57	149.00	124.40
1	A	94	ARG	CD-NE-CZ	14.74	145.04	124.40
2	O	353	HIS	CA-CB-CG	-12.42	101.38	113.80
1	A	87	ASN	CA-CB-CG	12.24	124.84	112.60
2	N	440	ARG	NE-CZ-NH2	-12.08	108.33	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	ARG	Sidechain
2	R	407	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	62	0
1	B	1571	0	1499	50	0
1	C	1571	0	1499	64	0
1	D	1571	0	1499	45	0
1	E	1571	0	1499	72	0
1	F	1571	0	1499	79	0
2	M	1840	0	1793	64	0
2	N	1840	0	1793	45	0
2	O	1840	0	1793	58	0
2	P	1840	0	1793	52	0
2	Q	1840	0	1793	61	0
2	R	1840	0	1793	73	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	4	0	5	0	0
4	N	4	0	5	1	0
4	O	4	0	5	0	0
4	P	4	0	5	0	0
4	Q	4	0	5	0	0
4	R	4	0	5	0	0
5	M	11	0	3	0	0
5	N	11	0	3	1	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	79	0	0	1	0
6	B	78	0	0	1	0
6	C	76	0	0	2	0
6	D	79	0	0	0	0
6	E	81	0	0	0	0
6	F	75	0	0	1	0
6	M	155	0	0	3	0
6	N	163	0	0	5	0
6	O	158	0	0	6	0
6	P	149	0	0	5	0
6	Q	160	0	0	6	0
6	R	163	0	0	4	0
All	All	21978	0	19800	645	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 16.

The worst 5 of 645 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	1.34	1.22
1:E:165:GLN:H	1:E:165:GLN:NE2	1.36	1.21
1:E:165:GLN:HE21	1:E:165:GLN:N	1.40	1.16
2:R:497:ASN:ND2	2:R:499:GLU:H	1.48	1.11
1:A:134:GLY:CA	2:M:326:THR:HG22	1.88	1.03

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%)	188 (95%)	10 (5%)	0	100	100
1	B	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	C	198/200 (99%)	189 (96%)	8 (4%)	1 (0%)	24	19
1	D	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	188 (95%)	9 (4%)	1 (0%)	24	19
2	M	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	N	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	224 (98%)	5 (2%)	0	100	100
2	Q	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	R	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
All	All	2562/2628 (98%)	2456 (96%)	104 (4%)	2 (0%)	48	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	101	ALA
1	F	74	ASP

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	14
1	B	162/163 (99%)	151 (93%)	11 (7%)	14	9
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	23
1	D	162/163 (99%)	155 (96%)	7 (4%)	26	23
1	E	162/163 (99%)	154 (95%)	8 (5%)	22	18
1	F	162/163 (99%)	155 (96%)	7 (4%)	26	23
2	M	196/202 (97%)	182 (93%)	14 (7%)	13	8
2	N	196/202 (97%)	189 (96%)	7 (4%)	31	30
2	O	196/202 (97%)	184 (94%)	12 (6%)	17	12
2	P	196/202 (97%)	186 (95%)	10 (5%)	21	17
2	Q	196/202 (97%)	186 (95%)	10 (5%)	21	17
2	R	196/202 (97%)	186 (95%)	10 (5%)	21	17
All	All	2148/2190 (98%)	2036 (95%)	112 (5%)	21	16

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	442	ILE
2	R	497	ASN
2	P	434	ASP
2	R	478	LEU
1	F	165	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	334	GLN
1	E	18	HIS
2	R	361	HIS
2	P	361	HIS
2	P	503	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
4	BME	M	601	2	3,3,3	0.68	0	2,2,2	1.04	0
5	INO	Q	550	3	10,11,11	1.81	4 (40%)	10,15,15	0.99	1 (10%)
5	INO	R	550	3	10,11,11	1.90	3 (30%)	10,15,15	0.98	1 (10%)
4	BME	Q	601	2	3,3,3	0.97	0	2,2,2	1.06	0
4	BME	N	601	2	3,3,3	0.62	0	2,2,2	1.31	0
4	BME	O	601	2	3,3,3	0.54	0	2,2,2	0.73	0
5	INO	M	550	3	10,11,11	1.91	4 (40%)	10,15,15	1.27	2 (20%)
5	INO	P	550	3	10,11,11	1.76	3 (30%)	10,15,15	1.07	1 (10%)
4	BME	R	601	2	3,3,3	0.41	0	2,2,2	0.71	0
5	INO	N	550	3	10,11,11	1.86	4 (40%)	10,15,15	1.07	1 (10%)
4	BME	P	601	2	3,3,3	0.79	0	2,2,2	1.63	1 (50%)
5	INO	O	550	3	10,11,11	1.73	3 (30%)	10,15,15	0.98	0

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
4	BME	M	601	2	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	INO	Q	550	3	-	0/4/4/4	0/1/1/1
5	INO	R	550	3	-	0/4/4/4	0/1/1/1
4	BME	Q	601	2	-	1/1/1/1	-
4	BME	N	601	2	-	1/1/1/1	-
4	BME	O	601	2	-	0/1/1/1	-
5	INO	M	550	3	-	0/4/4/4	0/1/1/1
5	INO	P	550	3	-	0/4/4/4	0/1/1/1
4	BME	R	601	2	-	1/1/1/1	-
5	INO	N	550	3	-	0/4/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-
5	INO	O	550	3	-	0/4/4/4	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	550	INO	O3-C2	-3.45	1.23	1.32
5	N	550	INO	O3-C2	-3.28	1.23	1.32
5	M	550	INO	O3-C2	-3.21	1.24	1.32
5	P	550	INO	O3-C2	-3.11	1.24	1.32
5	Q	550	INO	C3-C4	2.91	1.43	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	550	INO	O2-C7-C4	2.69	121.73	114.84
4	P	601	BME	O1-C1-C2	-2.30	101.85	110.82
5	R	550	INO	O2-C7-O1	-2.16	118.72	123.35
5	M	550	INO	O2-C7-O1	-2.12	118.80	123.35
5	Q	550	INO	O2-C7-C4	2.09	120.20	114.84

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	601	BME	O1-C1-C2-S2
4	Q	601	BME	O1-C1-C2-S2
4	R	601	BME	O1-C1-C2-S2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	601	BME	1	0
5	N	550	INO	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.