



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 12:18 AM UTC

PDB ID : 2PCD / pdb_00002pcd
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE FROM
PSEUDOMONAS AERUGINOSA AT 2.15 ANGSTROMS RESOLUTION
Authors : Ohlendorf, D.H.; Orville, A.M.; Lipscomb, J.D.
Deposited on : 1994-06-21
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
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

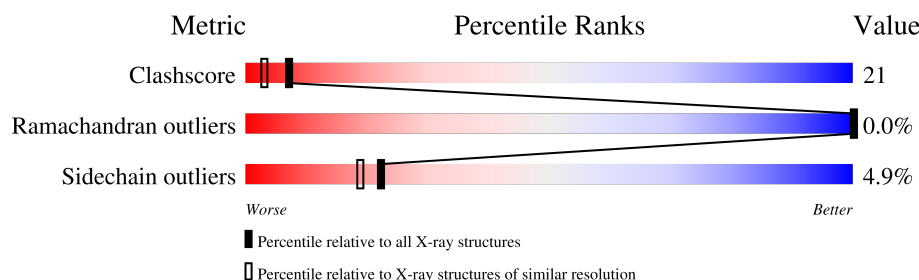
1 Overall quality at a glance

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	28% 51% 18% .
1	B	200	34% 46% 20%
1	C	200	26% 53% 20% .
1	D	200	32% 48% 20% .
1	E	200	25% 51% 22% .
1	F	200	27% 44% 26% .
2	M	238	30% 50% 15% . .
2	N	238	34% 48% 15% . .

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Mol	Chain	Length	Quality of chain
2	O	238	<div><div></div><div>38%42%16%<div><div></div><div></div></div></div></div>
2	P	238	<div><div></div><div>26%46%24%<div><div></div><div></div></div></div></div>
2	Q	238	<div><div></div><div>34%40%23%<div><div></div><div></div></div></div></div>
2	R	238	<div><div></div><div>30%42%24%<div><div></div><div></div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21906 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 (ALPHA CHAIN).

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 (BETA CHAIN).

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 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 water.

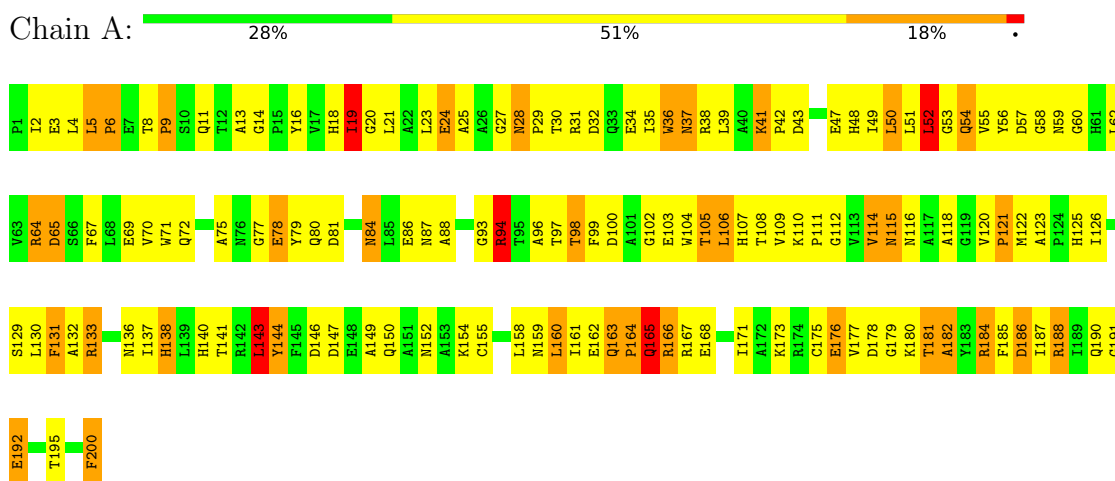
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	M	154	Total O 154 154	0	0
4	B	79	Total O 79 79	0	0
4	N	163	Total O 163 163	0	0
4	C	80	Total O 80 80	0	0
4	O	158	Total O 158 158	0	0
4	D	77	Total O 77 77	0	0
4	P	159	Total O 159 159	0	0
4	E	77	Total O 77 77	0	0
4	Q	163	Total O 163 163	0	0
4	F	83	Total O 83 83	0	0
4	R	158	Total O 158 158	0	0

3 Residue-property plots

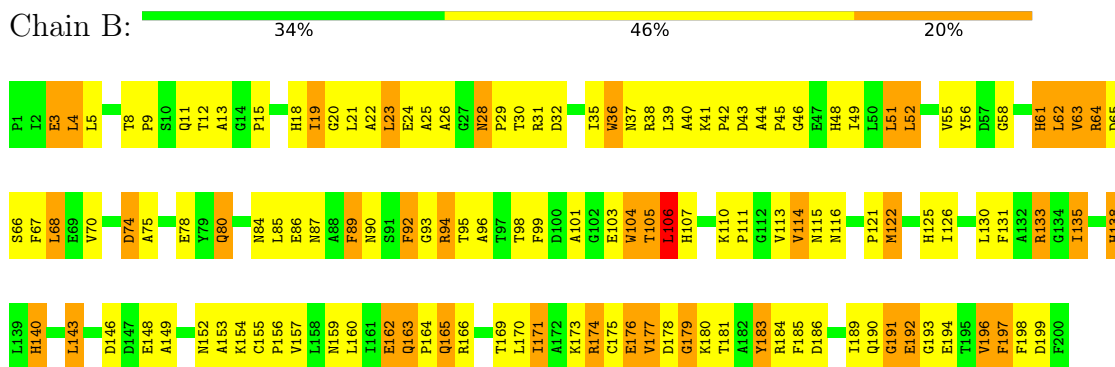
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

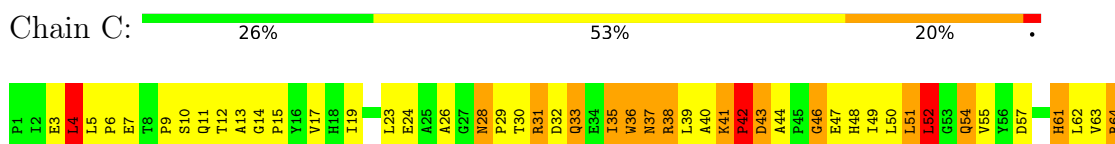
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)



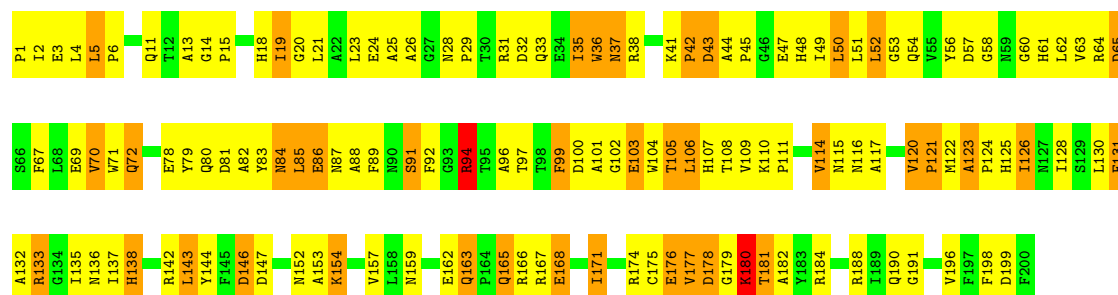
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)





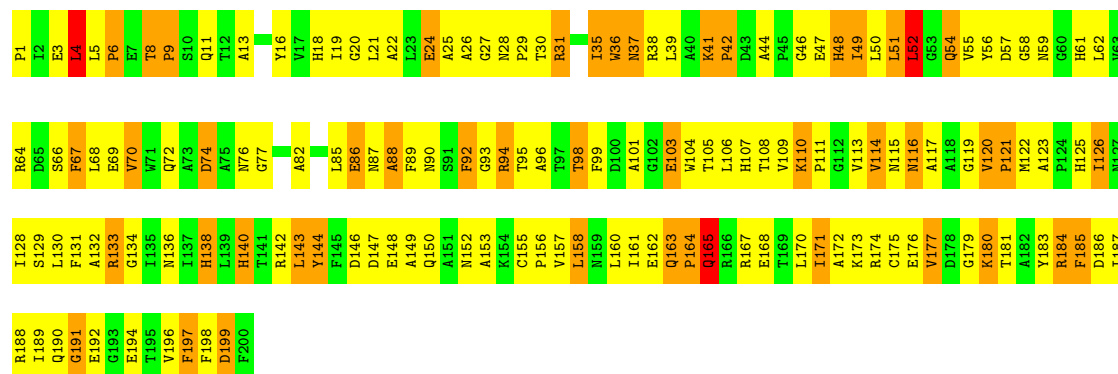
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain D: 32% 48% 20%



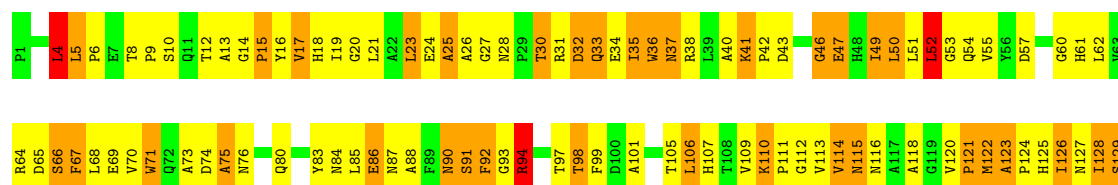
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

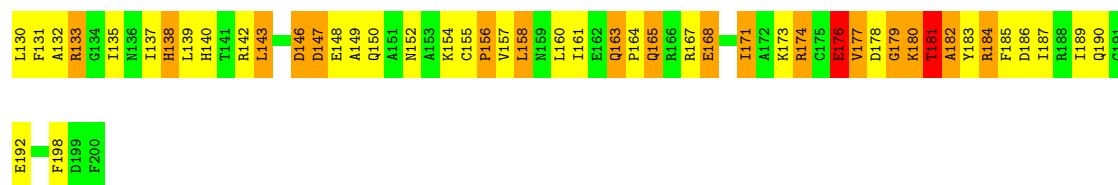
Chain E: 25% 51% 22%



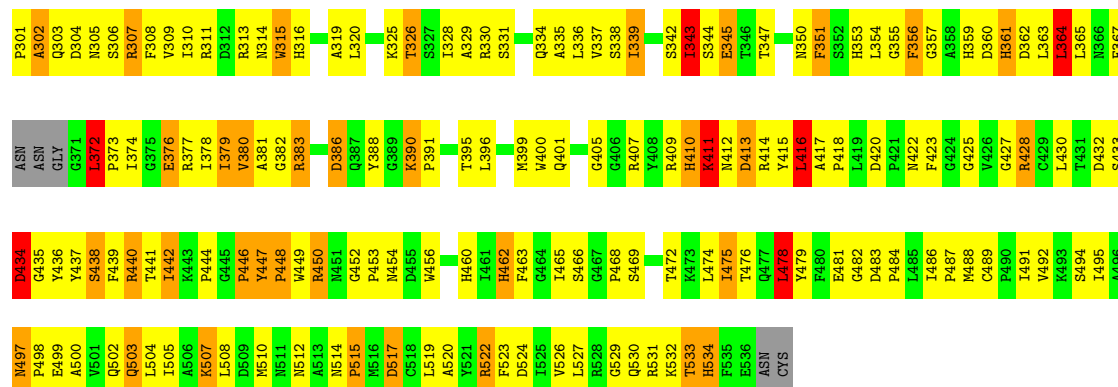
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain F: 27% 44% 26%

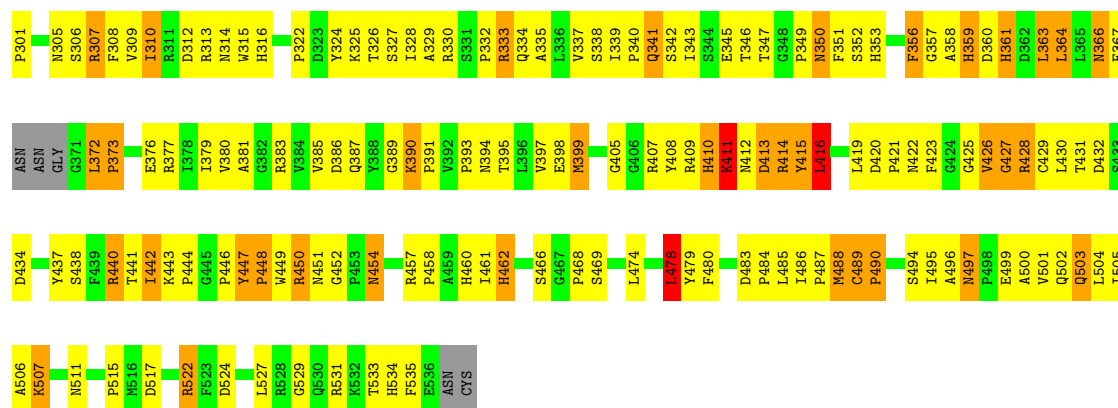
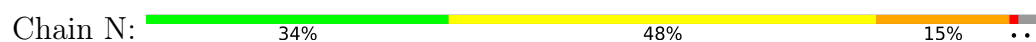




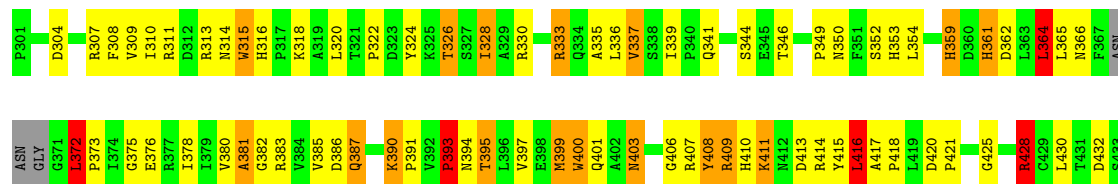
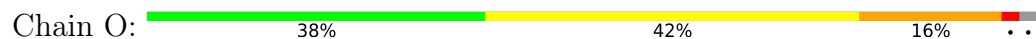
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

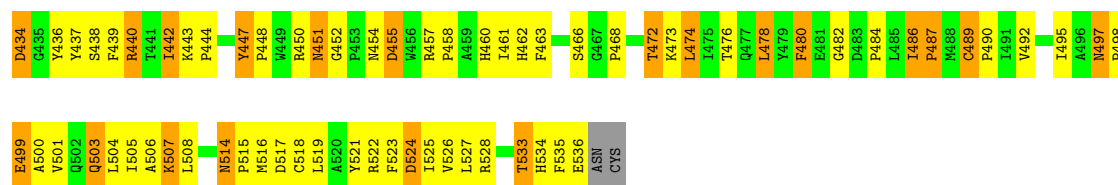


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

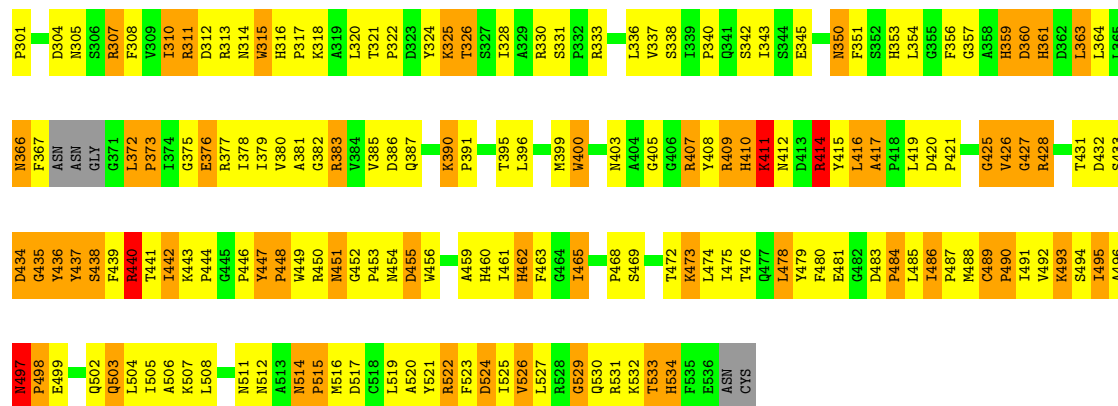


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

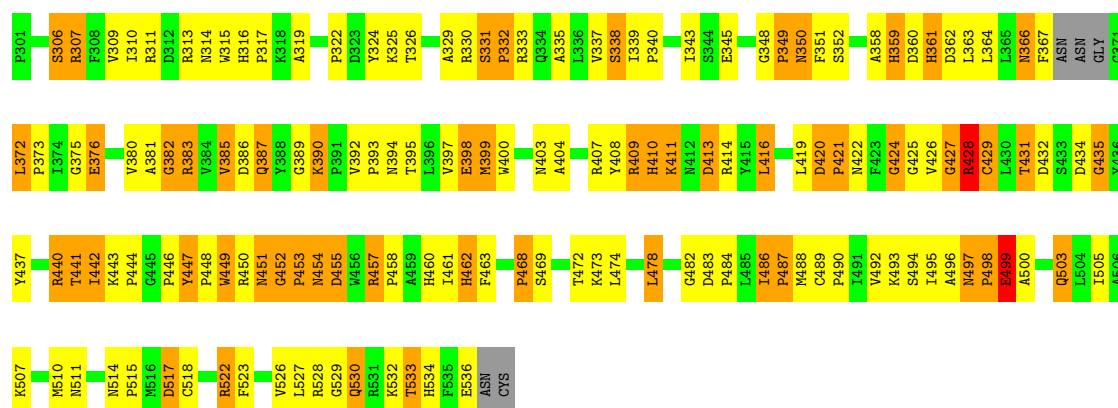
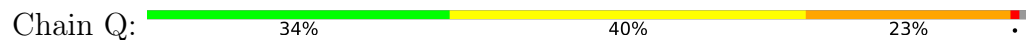




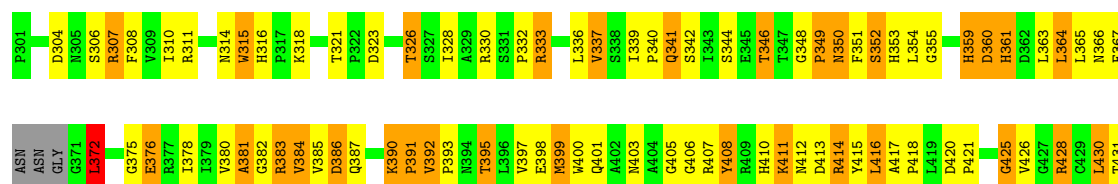
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)



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• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)



E469	A500	V501	Q502	Q503	E504	I505	A506	K507	L508	D509	E510	N511	N514	P515	M516	D517	L518	L519	A520	Y521	R522	F523	D524	I525	V526	L527	R528	Q529	Q530	R531	K532	T533	H534	F535	E536	ASN	CYS										
E449	A450	V451	Q452	Q453	E454	I455	A456	K457	L458	D459	E460	N461	N464	P465	M466	D467	L468	L469	A470	Y471	R472	F473	D474	I475	V476	L477	R478	Q479	Q480	E481	K482	D483	A484	L485	L486	P487	M488	D489	P490	L491	V492	K493	S494	L495	A496	P497	P498

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	197.17Å 127.03Å 134.18Å 90.00° 97.64° 90.00°	Depositor
Resolution (Å)	5.00 – 2.15	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21906	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: 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	2.53	116/1611 (7.2%)	2.20	64/2195 (2.9%)
1	B	2.54	95/1611 (5.9%)	2.11	60/2195 (2.7%)
1	C	2.40	89/1611 (5.5%)	2.23	75/2195 (3.4%)
1	D	2.55	104/1611 (6.5%)	2.16	52/2195 (2.4%)
1	E	2.58	118/1611 (7.3%)	2.17	69/2195 (3.1%)
1	F	2.42	91/1611 (5.6%)	2.20	54/2195 (2.5%)
2	M	2.47	106/1895 (5.6%)	2.21	70/2580 (2.7%)
2	N	2.54	120/1895 (6.3%)	2.15	65/2580 (2.5%)
2	O	2.41	96/1895 (5.1%)	2.12	63/2580 (2.4%)
2	P	2.54	115/1895 (6.1%)	2.23	76/2580 (2.9%)
2	Q	2.50	119/1895 (6.3%)	2.19	86/2580 (3.3%)
2	R	2.45	106/1895 (5.6%)	2.17	77/2580 (3.0%)
All	All	2.49	1275/21036 (6.1%)	2.18	811/28650 (2.8%)

The worst 5 of 1275 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	486	ILE	CA-CB	-10.85	1.48	1.54
2	Q	392	VAL	CA-CB	-10.83	1.44	1.54
2	P	460	HIS	CE1-NE2	-10.62	1.22	1.32
2	N	440	ARG	CD-NE	-10.41	1.31	1.46
1	E	133	ARG	NE-CZ	-10.37	1.21	1.33

The worst 5 of 811 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	38	ARG	CD-NE-CZ	19.08	151.11	124.40
1	A	94	ARG	CD-NE-CZ	15.77	146.48	124.40
2	N	434	ASP	CA-CB-CG	-15.02	97.58	112.60
2	N	440	ARG	NE-CZ-NH2	-14.03	106.58	119.20
1	C	94	ARG	CD-NE-CZ	13.27	142.97	124.40

There are no chirality outliers.

There are no planarity outliers.

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	61	0
1	B	1571	0	1499	72	0
1	C	1571	0	1499	75	0
1	D	1571	0	1499	50	0
1	E	1571	0	1499	69	0
1	F	1571	0	1499	101	0
2	M	1840	0	1793	85	0
2	N	1840	0	1793	62	0
2	O	1840	0	1793	64	0
2	P	1840	0	1793	93	0
2	Q	1840	0	1793	78	0
2	R	1840	0	1793	104	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	A	83	0	0	2	0
4	B	79	0	0	3	0
4	C	80	0	0	4	0
4	D	77	0	0	1	0
4	E	77	0	0	1	0
4	F	83	0	0	4	0
4	M	154	0	0	5	0
4	N	163	0	0	6	0
4	O	158	0	0	7	0
4	P	159	0	0	4	0
4	Q	163	0	0	8	0
4	R	158	0	0	8	0
All	All	21906	0	19752	838	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 21.

The worst 5 of 838 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:E:165:GLN:H	1:E:165:GLN:NE2	1.32	1.26
1:E:165:GLN:HE21	1:E:165:GLN:N	1.38	1.20
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.64	1.12
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.34	1.07
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.34	1.06

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%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	C	198/200 (99%)	192 (97%)	5 (2%)	1 (0%)	24	20
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%)	185 (93%)	13 (7%)	0	100	100
2	M	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	N	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	O	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	P	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	Q	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	R	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
All	All	2562/2628 (98%)	2463 (96%)	98 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	PRO

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%)	152 (94%)	10 (6%)	16	12
1	B	162/163 (99%)	155 (96%)	7 (4%)	26	24
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	24
1	D	162/163 (99%)	154 (95%)	8 (5%)	22	19
1	E	162/163 (99%)	157 (97%)	5 (3%)	35	37
1	F	162/163 (99%)	152 (94%)	10 (6%)	16	12
2	M	196/202 (97%)	186 (95%)	10 (5%)	21	18
2	N	196/202 (97%)	188 (96%)	8 (4%)	27	26
2	O	196/202 (97%)	185 (94%)	11 (6%)	19	15
2	P	196/202 (97%)	183 (93%)	13 (7%)	15	10
2	Q	196/202 (97%)	188 (96%)	8 (4%)	27	26
2	R	196/202 (97%)	188 (96%)	8 (4%)	27	26
All	All	2148/2190 (98%)	2043 (95%)	105 (5%)	22	19

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	94	ARG
2	P	497	ASN
2	R	416	LEU
1	D	165	GLN
2	P	416	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	165	GLN
1	E	107	HIS
2	R	361	HIS
2	P	361	HIS
2	P	497	ASN

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.