wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:36 AM GMT

PDB ID	:	3PCH
Title	:	STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COMPLEXED WITH 3-CHLORO-4-HYDROXYBENZOATE
Authors	:	Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1997-07-01
Resolution	:	2.05 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

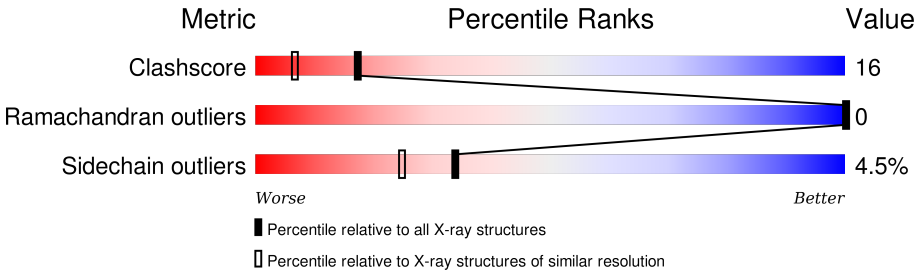
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.05 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	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	66% 29%
1	B	200	68% 28%
1	C	200	71% 25%
1	D	200	64% 32%
1	E	200	61% 34% 5%
1	F	200	64% 32%
2	M	238	63% 29% 5%

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Mol	Chain	Length	Quality of chain
2	N	238	69% 23% 5%
2	O	238	67% 27%
2	P	238	65% 28%
2	Q	238	62% 31%
2	R	238	67% 26% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22080 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			

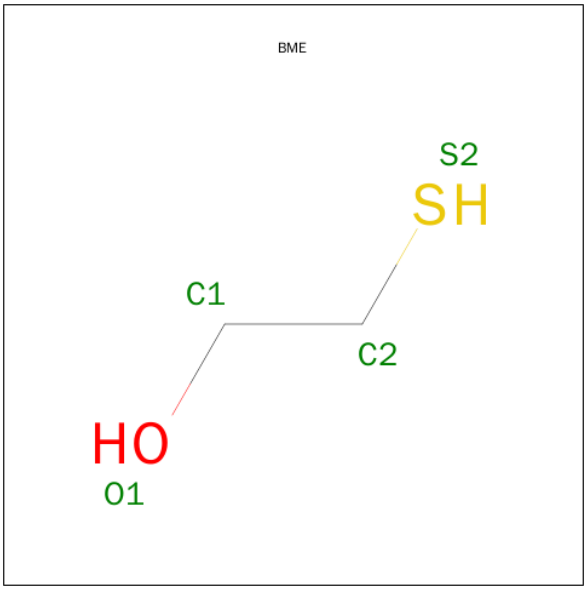
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

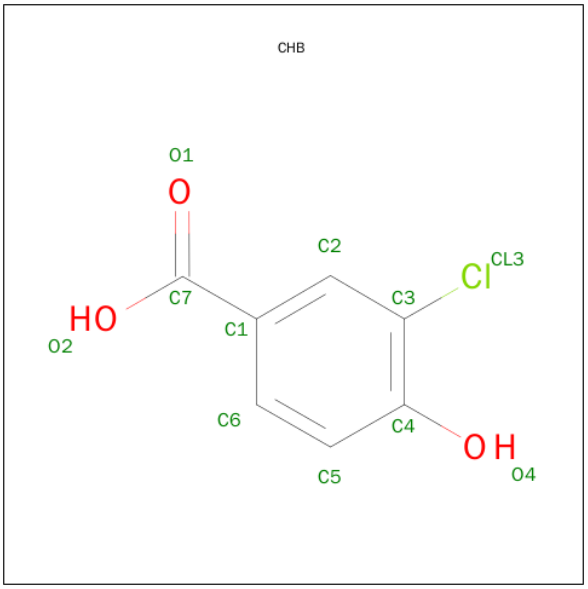
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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 3-CHLORO-4-HYDROXYBENZOIC ACID (three-letter code: CHB) (formula: $C_7H_5ClO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	M	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	N	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	N	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	O	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	O	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	P	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	P	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	Q	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	Q	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	R	1	Total	C	Cl	O	0	0
			11	7	1	3		
5	R	1	Total	C	Cl	O	0	0
			11	7	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	B	83	Total O 83 83	0	0
6	C	84	Total O 84 84	0	0
6	D	84	Total O 84 84	0	0
6	E	83	Total O 83 83	0	0
6	F	83	Total O 83 83	0	0
6	M	160	Total O 160 160	0	0
6	N	164	Total O 164 164	0	0
6	O	155	Total O 155 155	0	0
6	P	153	Total O 153 153	0	0
6	Q	163	Total O 163 163	0	0
6	R	158	Total O 158 158	0	0

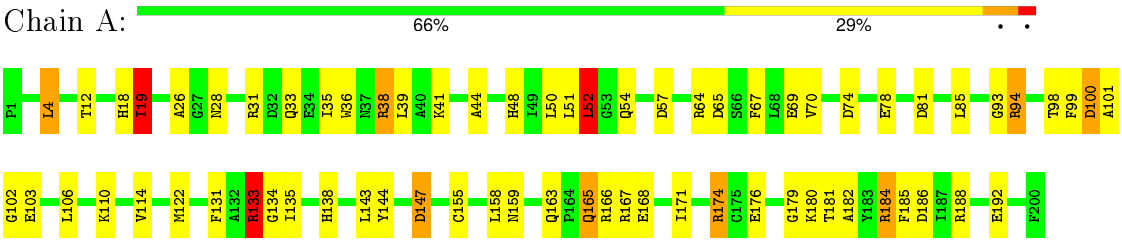
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

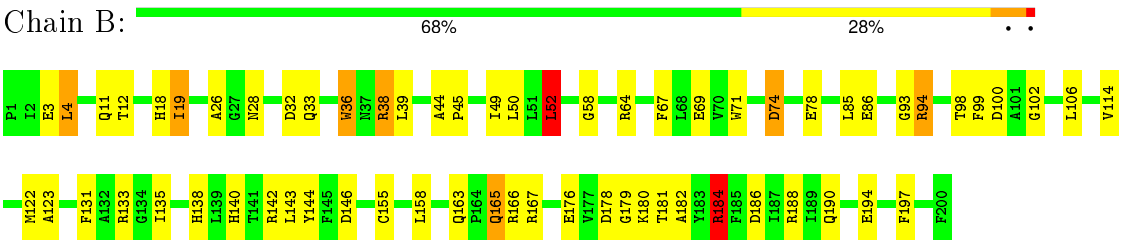
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A:



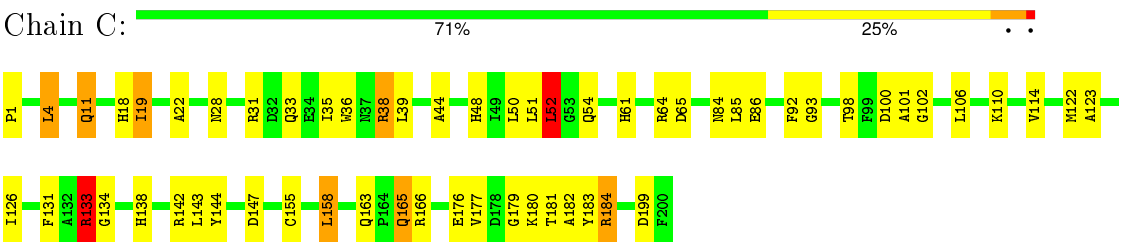
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B:



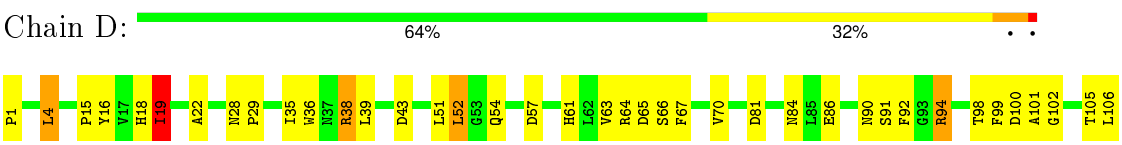
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

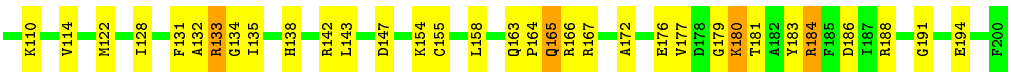
Chain C:



- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

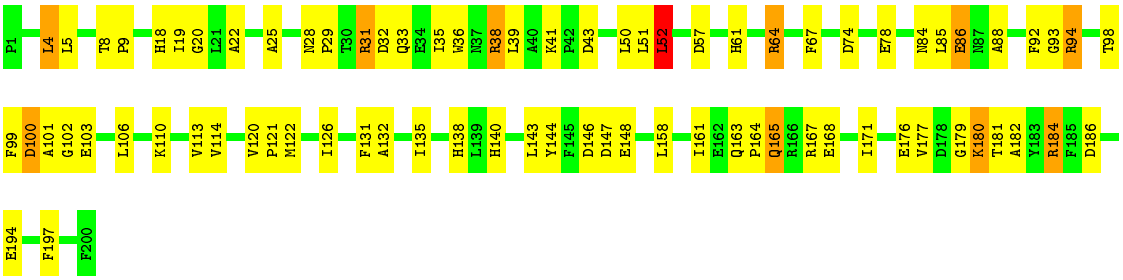
Chain D:





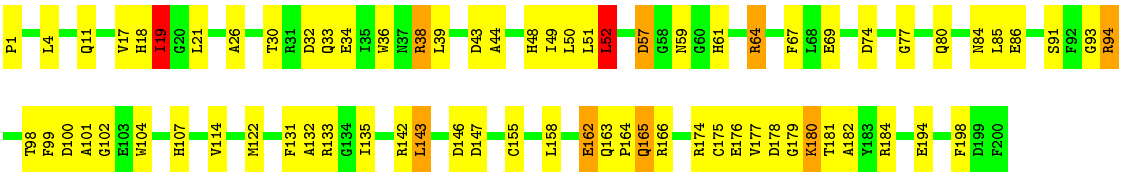
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:



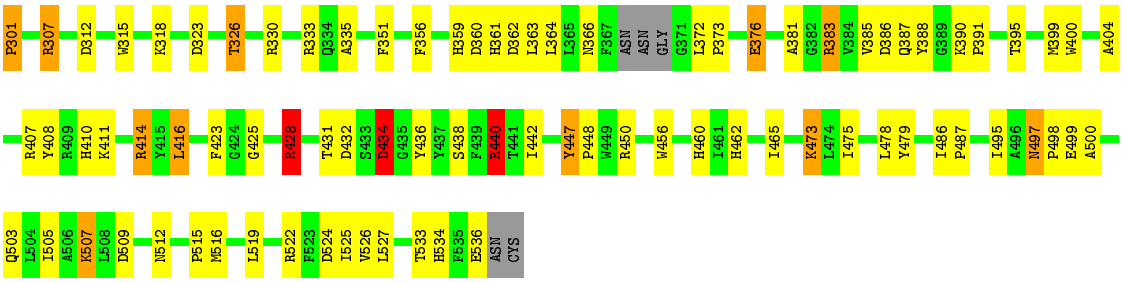
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:



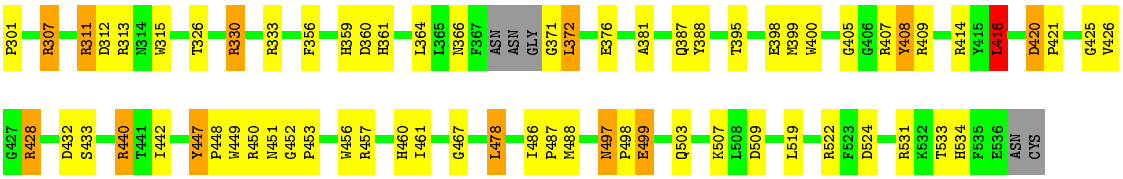
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:



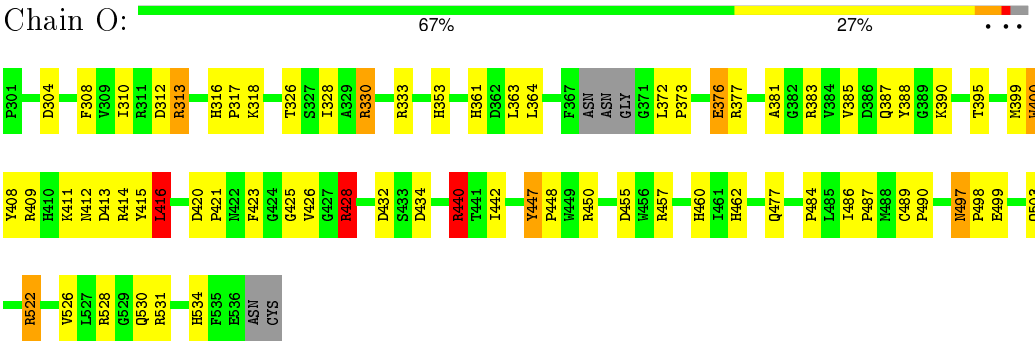
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N:



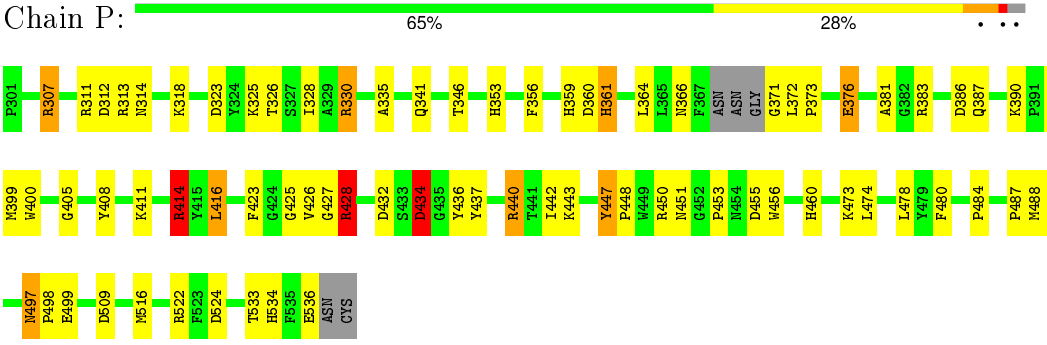
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:



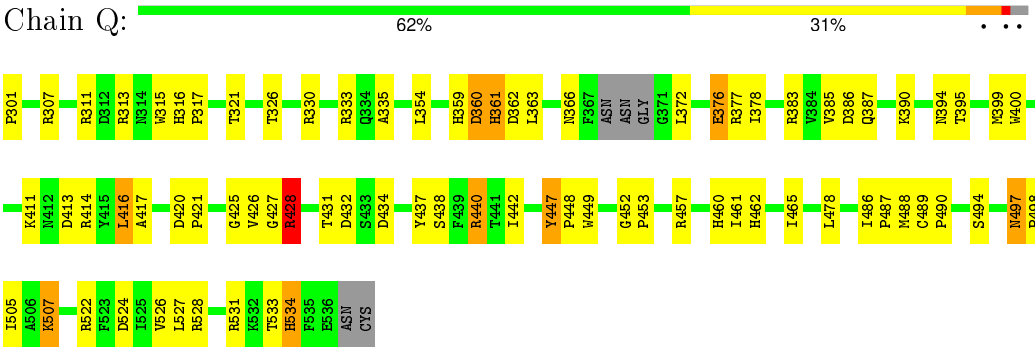
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



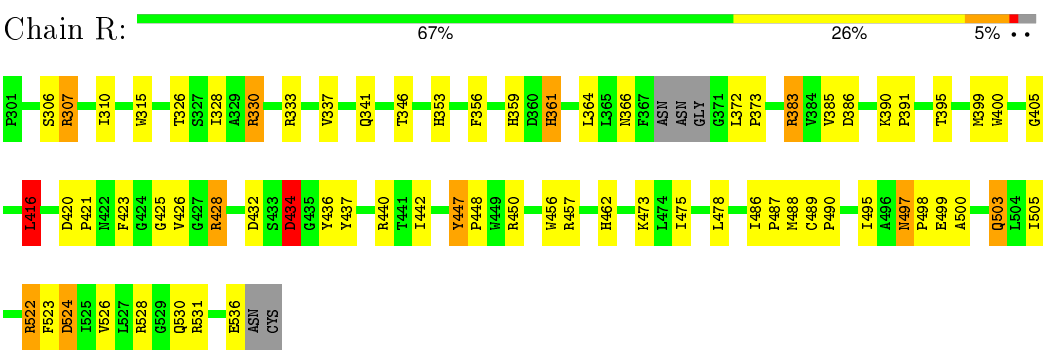
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:



4 Data and refinement statistics (i)

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, α, β, γ	195.39Å 126.52Å 133.33Å 90.00° 97.77° 90.00°	Depositor
Resolution (Å)	6.00 – 2.05	Depositor
% Data completeness (in resolution range)	75.2 (6.00-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22080	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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: CHB, FE, BME

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	1.00	1/1611 (0.1%)	1.71	27/2195 (1.2%)
1	B	1.04	2/1611 (0.1%)	1.79	30/2195 (1.4%)
1	C	0.97	0/1611	1.53	16/2195 (0.7%)
1	D	1.03	0/1611	1.70	23/2195 (1.0%)
1	E	1.02	1/1611 (0.1%)	1.59	20/2195 (0.9%)
1	F	1.02	1/1611 (0.1%)	1.68	28/2195 (1.3%)
2	M	1.10	2/1895 (0.1%)	1.75	35/2580 (1.4%)
2	N	1.11	4/1895 (0.2%)	1.65	38/2580 (1.5%)
2	O	1.11	1/1895 (0.1%)	1.68	38/2580 (1.5%)
2	P	1.08	2/1895 (0.1%)	1.77	35/2580 (1.4%)
2	Q	1.13	3/1895 (0.2%)	1.73	38/2580 (1.5%)
2	R	1.08	2/1895 (0.1%)	1.72	33/2580 (1.3%)
All	All	1.06	19/21036 (0.1%)	1.69	361/28650 (1.3%)

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	A	0	1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	428	ARG	CD-NE	-6.80	1.34	1.46
2	M	428	ARG	CD-NE	-6.51	1.35	1.46
2	Q	428	ARG	CD-NE	-6.50	1.35	1.46
1	B	94	ARG	CD-NE	-6.20	1.35	1.46
2	P	440	ARG	CD-NE	-5.92	1.36	1.46

The worst 5 of 361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	440	ARG	NE-CZ-NH2	-24.33	108.14	120.30
2	M	440	ARG	NE-CZ-NH2	-21.92	109.34	120.30
2	Q	440	ARG	NE-CZ-NH2	-21.33	109.64	120.30
2	P	440	ARG	NE-CZ-NH1	20.20	130.40	120.30
1	B	184	ARG	NE-CZ-NH2	-19.49	110.56	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain

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	56	0
1	B	1571	0	1499	53	0
1	C	1571	0	1499	57	0
1	D	1571	0	1499	58	0
1	E	1571	0	1499	64	0
1	F	1571	0	1499	71	0
2	M	1840	0	1792	77	0
2	N	1840	0	1792	43	0
2	O	1840	0	1792	57	0
2	P	1840	0	1792	67	0
2	Q	1840	0	1792	62	0
2	R	1840	0	1792	53	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	M	4	0	5	3	0
4	N	4	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	4	0	5	1	0
4	P	4	0	5	0	0
4	Q	4	0	5	2	0
4	R	4	0	5	0	0
5	M	22	0	7	2	0
5	N	22	0	7	2	0
5	O	22	0	6	2	0
5	P	22	0	7	0	0
5	Q	22	0	7	2	0
5	R	22	0	7	2	0
6	A	82	0	0	2	0
6	B	83	0	0	4	0
6	C	84	0	0	3	0
6	D	84	0	0	2	0
6	E	83	0	0	3	0
6	F	83	0	0	3	0
6	M	160	0	0	4	0
6	N	164	0	0	2	0
6	O	155	0	0	5	0
6	P	153	0	0	4	0
6	Q	163	0	0	4	0
6	R	158	0	0	2	0
All	All	22080	0	19817	651	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 651 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)
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.16	1.12
1:B:18:HIS:ND1	6:B:648:HOH:O	1.83	1.09
1:E:165:GLN:NE2	1:E:165:GLN:H	1.47	1.09
1:F:165:GLN:NE2	1:F:165:GLN:H	1.52	1.07
1:B:165:GLN:NE2	1:B:165:GLN:H	1.52	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%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	C	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	D	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	E	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	F	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
2	M	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	P	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	Q	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	R	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
All	All	2562/2628 (98%)	2480 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	156 (96%)	6 (4%)	41	32
1	B	162/163 (99%)	154 (95%)	8 (5%)	31	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	162/163 (99%)	156 (96%)	6 (4%)	41	32
1	D	162/163 (99%)	154 (95%)	8 (5%)	31	21
1	E	162/163 (99%)	155 (96%)	7 (4%)	35	27
1	F	162/163 (99%)	156 (96%)	6 (4%)	41	32
2	M	196/202 (97%)	185 (94%)	11 (6%)	26	16
2	N	196/202 (97%)	187 (95%)	9 (5%)	33	24
2	O	196/202 (97%)	187 (95%)	9 (5%)	33	24
2	P	196/202 (97%)	187 (95%)	9 (5%)	33	24
2	Q	196/202 (97%)	187 (95%)	9 (5%)	33	24
2	R	196/202 (97%)	188 (96%)	8 (4%)	37	28
All	All	2148/2190 (98%)	2052 (96%)	96 (4%)	34	25

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	428	ARG
1	D	91	SER
2	R	372	LEU
2	O	440	ARG
2	O	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	GLN
2	P	497	ASN
2	R	412	ASN
2	P	361	HIS
2	N	412	ASN

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 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	CHB	M	550	3	8,11,11	0.69	0	11,15,15	1.03	0
5	CHB	M	551	-	8,11,11	0.67	0	11,15,15	0.89	0
4	BME	M	601	2	3,3,3	0.33	0	2,2,2	0.24	0
5	CHB	N	550	3,2	8,11,11	0.62	0	11,15,15	1.12	0
5	CHB	N	551	-	8,11,11	0.94	0	11,15,15	0.88	0
4	BME	N	601	2	3,3,3	0.17	0	2,2,2	0.43	0
5	CHB	O	550	3	8,11,11	0.59	0	11,15,15	1.33	2 (18%)
5	CHB	O	551	-	8,11,11	0.76	0	11,15,15	1.08	1 (9%)
4	BME	O	601	2	3,3,3	0.42	0	2,2,2	0.54	0
5	CHB	P	550	3	8,11,11	0.68	0	11,15,15	1.07	0
5	CHB	P	551	-	8,11,11	0.95	0	11,15,15	0.67	0
4	BME	P	601	2	3,3,3	0.79	0	2,2,2	1.41	0
5	CHB	Q	550	3	8,11,11	0.60	0	11,15,15	1.35	2 (18%)
5	CHB	Q	551	-	8,11,11	0.69	0	11,15,15	0.93	0
4	BME	Q	601	2	3,3,3	0.63	0	2,2,2	0.77	0
5	CHB	R	550	3,2	8,11,11	0.60	0	11,15,15	0.93	0
5	CHB	R	551	-	8,11,11	0.63	0	11,15,15	0.66	0
4	BME	R	601	2	3,3,3	0.64	0	2,2,2	1.09	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
5	CHB	M	550	3	-	0/0/4/4	0/1/1/1
5	CHB	M	551	-	-	0/0/4/4	0/1/1/1
4	BME	M	601	2	-	0/1/1/1	0/0/0/0
5	CHB	N	550	3,2	-	0/0/4/4	0/1/1/1
5	CHB	N	551	-	-	0/0/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	0/0/0/0
5	CHB	O	550	3	-	0/0/4/4	0/1/1/1
5	CHB	O	551	-	-	0/0/4/4	0/1/1/1
4	BME	O	601	2	-	0/1/1/1	0/0/0/0
5	CHB	P	550	3	-	0/0/4/4	0/1/1/1
5	CHB	P	551	-	-	0/0/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	0/0/0/0
5	CHB	Q	550	3	-	0/0/4/4	0/1/1/1
5	CHB	Q	551	-	-	0/0/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	0/0/0/0
5	CHB	R	550	3,2	-	0/0/4/4	0/1/1/1
5	CHB	R	551	-	-	0/0/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	550	CHB	C2-C3-C4	-2.70	119.72	121.22
5	O	550	CHB	C2-C3-C4	-2.35	119.91	121.22
5	O	551	CHB	C5-C4-C3	2.02	120.62	118.57
5	Q	550	CHB	C5-C4-C3	2.33	120.94	118.57
5	O	550	CHB	C5-C4-C3	2.51	121.12	118.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	550	CHB	2	0
4	M	601	BME	3	0
5	N	550	CHB	2	0
5	O	550	CHB	2	0
4	O	601	BME	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	550	CHB	2	0
4	Q	601	BME	2	0
5	R	550	CHB	2	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 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.