



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:47 PM GMT

PDB ID : 1YKM
Title : Protocatechuate 3,4-Dioxygenase Y408E mutant
Authors : Brown, C.K.; Ohlendorf, D.H.
Deposited on : 2005-01-18
Resolution : 2.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

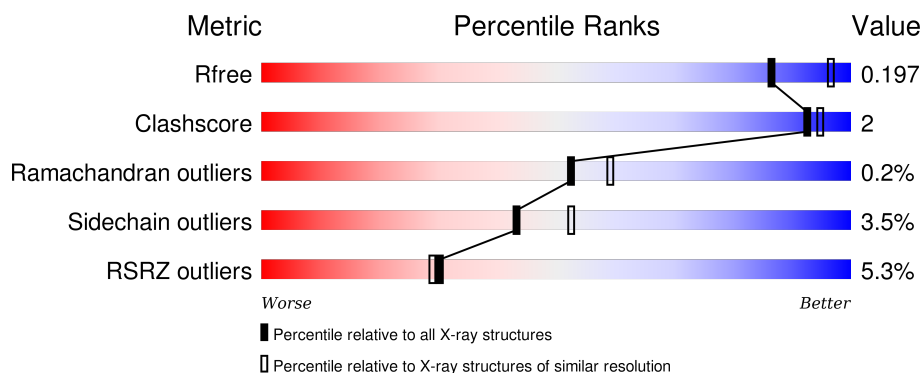
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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))
R_{free}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	200	<div> <div>6%</div> <div>95%</div> <div>• •</div> </div>
1	C	200	<div> <div>7%</div> <div>95%</div> <div>• •</div> </div>
1	E	200	<div> <div>5%</div> <div>94%</div> <div>6% •</div> </div>
1	G	200	<div> <div>7%</div> <div>95%</div> <div>• •</div> </div>
1	I	200	<div> <div>8%</div> <div>94%</div> <div>5% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	200	<div><div></div><div>9%</div><div></div><div>94%</div><div></div><div>5%</div><div></div></div>
2	B	238	<div><div></div><div>4%</div><div></div><div>94%</div><div></div><div>5%</div><div></div></div>
2	D	238	<div><div></div><div>4%</div><div></div><div>92%</div><div></div><div>7%</div><div></div></div>
2	F	238	<div><div></div><div>3%</div><div></div><div>92%</div><div></div><div>6%</div><div></div></div>
2	H	238	<div><div></div><div>3%</div><div></div><div>91%</div><div></div><div>8%</div><div></div></div>
2	J	238	<div><div></div><div>5%</div><div></div><div>95%</div><div></div><div></div><div></div></div>
2	L	238	<div><div></div><div>5%</div><div></div><div>94%</div><div></div><div>5%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22002 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	C	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	G	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	I	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	K	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	B	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	D	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	F	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	H	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	J	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	L	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	GLU	TYR	ENGINEERED	UNP P00437

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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
D	408	GLU	TYR	ENGINEERED	UNP P00437
D	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
F	408	GLU	TYR	ENGINEERED	UNP P00437
F	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
H	408	GLU	TYR	ENGINEERED	UNP P00437
H	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
J	408	GLU	TYR	ENGINEERED	UNP P00437
J	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
L	408	GLU	TYR	ENGINEERED	UNP P00437
L	429	CME	CYS	MODIFIED RESIDUE	UNP P00437

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	H	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	L	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	140	Total O 140 140	0	0
4	C	78	Total O 78 78	0	0
4	D	146	Total O 146 146	0	0
4	E	76	Total O 76 76	0	0
4	F	141	Total O 141 141	0	0

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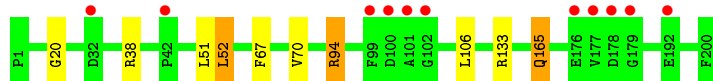
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	77	Total 77	O 77	0	0
4	H	137	Total 137	O 137	0	0
4	I	75	Total 75	O 75	0	0
4	J	147	Total 147	O 147	0	0
4	K	78	Total 78	O 78	0	0
4	L	141	Total 141	O 141	0	0

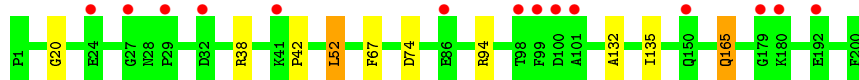
3 Residue-property plots [i](#)

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.

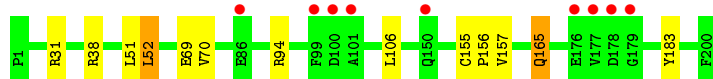
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



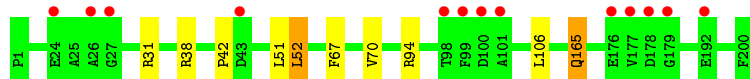
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



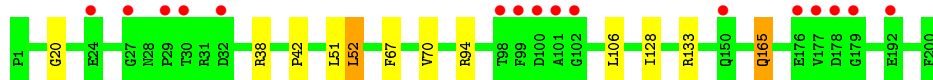
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



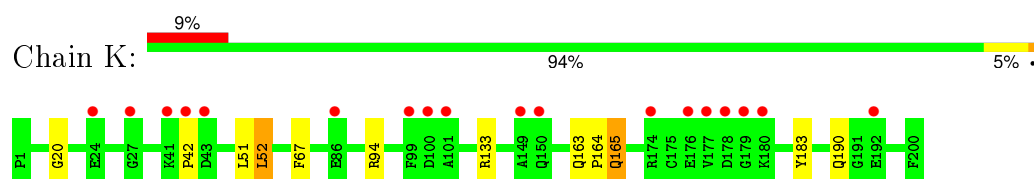
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



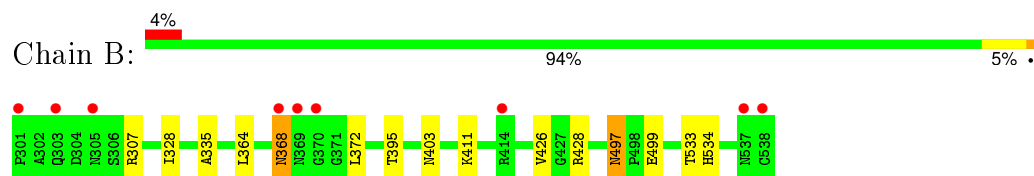
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



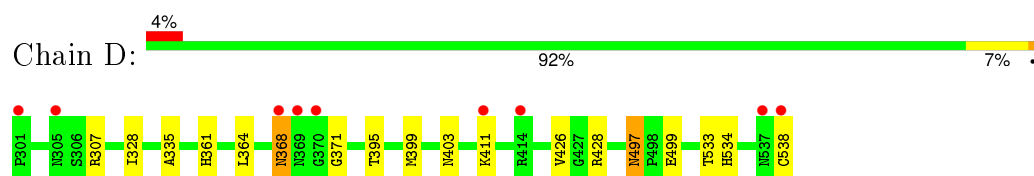
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



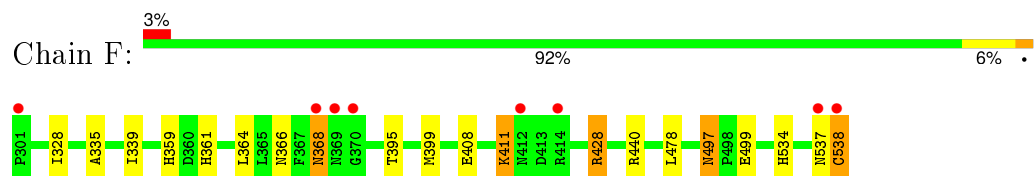
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



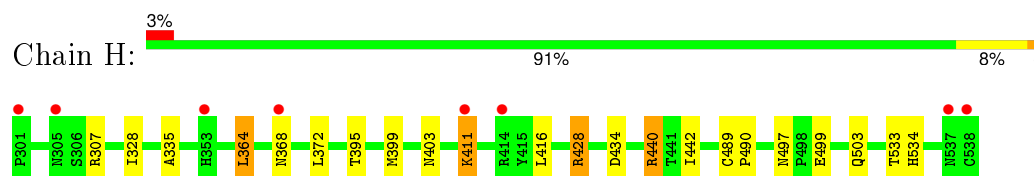
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



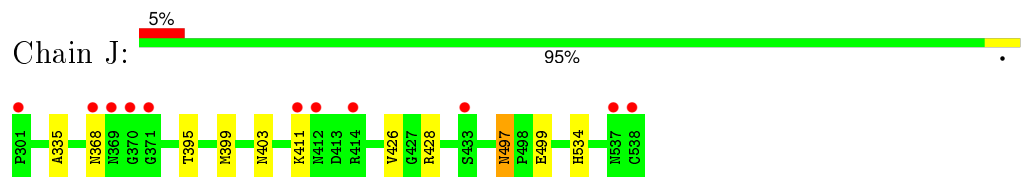
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



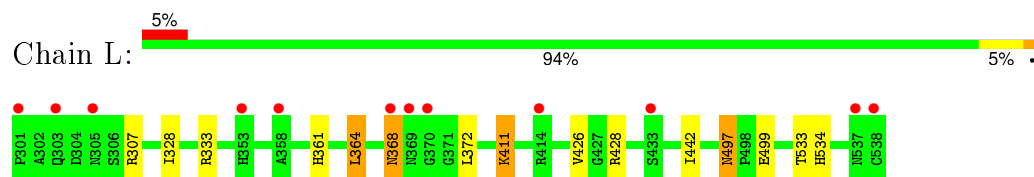
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.61Å 127.73Å 134.32Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	7.81 – 2.22 19.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	69.4 (7.81-2.22) 68.0 (19.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.94Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.169 , 0.199 0.169 , 0.197	Depositor DCC
R_{free} test set	1443 reflections (1.32%)	DCC
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 195111 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22002	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CME, 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	0.62	0/1611	0.75	1/2195 (0.0%)
1	C	0.61	0/1611	0.74	1/2195 (0.0%)
1	E	0.63	0/1611	0.74	1/2195 (0.0%)
1	G	0.63	0/1611	0.75	1/2195 (0.0%)
1	I	0.64	0/1611	0.74	1/2195 (0.0%)
1	K	0.63	0/1611	0.73	1/2195 (0.0%)
2	B	0.61	0/1920	0.78	0/2612
2	D	0.61	0/1920	0.78	0/2612
2	F	0.61	0/1920	0.77	0/2612
2	H	0.62	0/1920	0.76	1/2612 (0.0%)
2	J	0.63	0/1920	0.76	0/2612
2	L	0.62	0/1920	0.77	0/2612
All	All	0.62	0/21186	0.76	7/28842 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	52	LEU	CA-CB-CG	7.61	132.80	115.30
1	A	52	LEU	CA-CB-CG	7.48	132.50	115.30
1	E	52	LEU	CA-CB-CG	7.44	132.40	115.30
1	G	52	LEU	CA-CB-CG	7.19	131.84	115.30
1	I	52	LEU	CA-CB-CG	6.94	131.27	115.30
1	C	52	LEU	CA-CB-CG	6.19	129.53	115.30
2	H	416	LEU	CA-CB-CG	5.27	127.43	115.30

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	6	0
1	C	1571	0	1499	7	0
1	E	1571	0	1499	8	0
1	G	1571	0	1499	7	0
1	I	1571	0	1499	9	0
1	K	1571	0	1499	8	0
2	B	1876	0	1820	6	0
2	D	1876	0	1820	9	0
2	F	1876	0	1820	11	0
2	H	1876	0	1820	10	0
2	J	1876	0	1820	4	0
2	L	1876	0	1820	8	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	A	78	0	0	0	0
4	B	140	0	0	1	0
4	C	78	0	0	1	0
4	D	146	0	0	1	0
4	E	76	0	0	0	0
4	F	141	0	0	0	0
4	G	77	0	0	0	0
4	H	137	0	0	1	0
4	I	75	0	0	0	0
4	J	147	0	0	1	0
4	K	78	0	0	0	0
4	L	141	0	0	0	0
All	All	22002	0	19914	79	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 2.

All (79) 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:I:165:GLN:H	1:I:165:GLN:HE21	1.07	1.00
1:C:165:GLN:H	1:C:165:GLN:HE21	1.16	0.92
1:G:165:GLN:HE21	1:G:165:GLN:H	1.36	0.71
1:I:165:GLN:N	1:I:165:GLN:HE21	1.90	0.59
1:I:51:LEU:HD12	1:I:106:LEU:HD23	1.85	0.59
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.68	0.59
2:F:411:LYS:HZ2	2:F:411:LYS:H	1.49	0.58
1:G:51:LEU:HD12	1:G:106:LEU:HD23	1.85	0.58
1:I:165:GLN:H	1:I:165:GLN:NE2	1.90	0.57
2:H:335:ALA:HB2	2:L:328:ILE:HD12	1.88	0.56
2:L:307:ARG:HG2	2:L:533:THR:HG22	1.90	0.54
2:J:497:ASN:HD22	2:J:499:GLU:H	1.56	0.53
2:D:307:ARG:HG2	2:D:533:THR:HG22	1.90	0.53
1:K:67:PHE:HZ	1:K:94:ARG:HD2	1.73	0.53
1:E:165:GLN:NE2	1:E:165:GLN:H	2.07	0.53
2:H:364:LEU:HD22	2:H:440:ARG:HD3	1.91	0.53
1:C:20:GLY:HA2	2:D:426:VAL:HG13	1.89	0.52
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.73	0.52
2:D:497:ASN:HD22	2:D:499:GLU:H	1.58	0.52
1:G:67:PHE:HZ	1:G:94:ARG:HD2	1.73	0.52
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.91	0.52
1:G:165:GLN:NE2	1:G:165:GLN:H	2.05	0.51
2:F:497:ASN:HD22	2:F:499:GLU:H	1.58	0.51
2:B:335:ALA:HB2	2:F:328:ILE:HD12	1.93	0.50
1:I:20:GLY:HA2	2:J:426:VAL:HG13	1.93	0.49
1:A:51:LEU:HD12	1:A:106:LEU:HD23	1.94	0.49
1:A:20:GLY:HA2	2:B:426:VAL:HG13	1.95	0.48
1:K:165:GLN:NE2	1:K:165:GLN:H	2.11	0.48
2:D:538:CYS:HA	2:H:440:ARG:HH22	1.78	0.48
1:A:165:GLN:H	1:A:165:GLN:NE2	2.10	0.48
1:I:67:PHE:HZ	1:I:94:ARG:HD2	1.78	0.48
2:B:307:ARG:HG2	2:B:533:THR:HG22	1.95	0.48
2:H:328:ILE:HD12	2:J:335:ALA:HB2	1.96	0.48
1:C:165:GLN:N	1:C:165:GLN:HE21	1.98	0.48
2:D:328:ILE:HD12	2:F:335:ALA:HB2	1.94	0.47
2:H:411:LYS:H	2:H:411:LYS:NZ	2.13	0.47
2:F:411:LYS:NZ	2:F:411:LYS:H	2.13	0.46
2:H:307:ARG:HG2	2:H:533:THR:HG22	1.97	0.46
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.98	0.46
1:K:67:PHE:CZ	1:K:94:ARG:HD2	2.50	0.46
1:G:67:PHE:CZ	1:G:94:ARG:HD2	2.51	0.46
1:I:70:VAL:HG21	1:I:106:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ASN:HD22	2:B:499:GLU:H	1.64	0.45
2:L:497:ASN:HD22	2:L:499:GLU:H	1.64	0.45
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.50	0.44
2:F:537:ASN:O	2:F:538:CYS:HB2	2.17	0.44
2:F:364:LEU:HD22	2:F:440:ARG:HD3	2.00	0.44
1:K:163:GLN:HA	1:K:164:PRO:HD2	1.90	0.44
1:G:31:ARG:NH1	2:H:428:ARG:HG2	2.32	0.44
1:E:31:ARG:NH1	2:F:428:ARG:HG2	2.32	0.44
1:C:132:ALA:HB3	1:C:135:ILE:HD12	2.00	0.44
2:D:368:ASN:ND2	2:D:371:GLY:H	2.16	0.43
2:D:403:ASN:HB2	4:D:1620:HOH:O	2.18	0.43
2:L:411:LYS:HZ3	2:L:411:LYS:H	1.66	0.43
2:J:403:ASN:HB2	4:J:4620:HOH:O	2.17	0.43
2:L:361:HIS:CD2	2:L:361:HIS:H	2.36	0.43
2:H:403:ASN:HB2	4:H:3620:HOH:O	2.18	0.43
2:L:364:LEU:HD11	2:L:442:ILE:HG23	2.01	0.43
1:E:69:GLU:HG2	1:E:94:ARG:HG2	2.00	0.43
2:B:328:ILE:HD12	2:D:335:ALA:HB2	1.99	0.42
2:D:361:HIS:CD2	2:D:361:HIS:H	2.37	0.42
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.52	0.42
1:I:67:PHE:CZ	1:I:94:ARG:HD2	2.54	0.42
2:F:359:HIS:O	2:F:366:ASN:HB3	2.19	0.42
1:K:165:GLN:HE21	1:K:165:GLN:H	1.67	0.42
1:K:51:LEU:HD23	1:K:183:TYR:HB2	2.01	0.42
2:H:489:CYS:HA	2:H:490:PRO:HD3	1.92	0.41
2:H:364:LEU:HD11	2:H:442:ILE:HG23	2.02	0.41
1:G:70:VAL:HG21	1:G:106:LEU:HD21	2.03	0.41
1:E:51:LEU:HD23	1:E:183:TYR:HB2	2.03	0.41
1:E:155:CYS:HA	1:E:156:PRO:HD3	1.95	0.41
1:E:157:VAL:HG13	2:F:339:ILE:HG21	2.03	0.41
1:K:20:GLY:HA2	2:L:426:VAL:HG13	2.03	0.41
2:F:361:HIS:H	2:F:361:HIS:CD2	2.38	0.41
1:E:70:VAL:HG21	1:E:106:LEU:HD21	2.02	0.41
1:C:74:ASP:HB2	4:C:1690:HOH:O	2.21	0.40
1:I:70:VAL:HG12	1:I:128:ILE:HG12	2.02	0.40
2:B:403:ASN:HB2	4:B:620:HOH:O	2.21	0.40
1:K:190:GLN:HG3	2:L:333:ARG:HG2	2.04	0.40

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%)	193 (98%)	5 (2%)	0	100	100
1	C	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	E	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	G	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	I	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	K	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
2	B	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	39	41
2	D	235/238 (99%)	229 (97%)	5 (2%)	1 (0%)	39	41
2	F	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	39	41
2	H	235/238 (99%)	228 (97%)	7 (3%)	0	100	100
2	J	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	39	41
2	L	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	39	41
All	All	2598/2628 (99%)	2519 (97%)	74 (3%)	5 (0%)	52	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	368	ASN
2	D	368	ASN
2	F	368	ASN
2	J	368	ASN
2	L	368	ASN

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%)	157 (97%)	5 (3%)	47	58
1	C	162/163 (99%)	158 (98%)	4 (2%)	55	67
1	E	162/163 (99%)	159 (98%)	3 (2%)	65	77
1	G	162/163 (99%)	158 (98%)	4 (2%)	55	67
1	I	162/163 (99%)	157 (97%)	5 (3%)	47	58
1	K	162/163 (99%)	158 (98%)	4 (2%)	55	67
2	B	199/201 (99%)	191 (96%)	8 (4%)	38	46
2	D	199/201 (99%)	192 (96%)	7 (4%)	43	52
2	F	199/201 (99%)	189 (95%)	10 (5%)	30	34
2	H	199/201 (99%)	186 (94%)	13 (6%)	21	22
2	J	199/201 (99%)	193 (97%)	6 (3%)	48	60
2	L	199/201 (99%)	192 (96%)	7 (4%)	43	52
All	All	2166/2184 (99%)	2090 (96%)	76 (4%)	43	52

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	52	LEU
1	A	94	ARG
1	A	133	ARG
1	A	165	GLN
2	B	364	LEU
2	B	368	ASN
2	B	372	LEU
2	B	395	THR
2	B	411	LYS
2	B	428	ARG
2	B	497	ASN
2	B	534	HIS
1	C	38	ARG
1	C	42	PRO
1	C	52	LEU
1	C	165	GLN
2	D	364	LEU
2	D	395	THR

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Mol	Chain	Res	Type
2	D	399	MET
2	D	411	LYS
2	D	428	ARG
2	D	497	ASN
2	D	534	HIS
1	E	38	ARG
1	E	52	LEU
1	E	165	GLN
2	F	368	ASN
2	F	395	THR
2	F	399	MET
2	F	408	GLU
2	F	411	LYS
2	F	428	ARG
2	F	478	LEU
2	F	497	ASN
2	F	534	HIS
2	F	538	CYS
1	G	38	ARG
1	G	42	PRO
1	G	52	LEU
1	G	165	GLN
2	H	364	LEU
2	H	368	ASN
2	H	372	LEU
2	H	395	THR
2	H	399	MET
2	H	411	LYS
2	H	428	ARG
2	H	434	ASP
2	H	440	ARG
2	H	497	ASN
2	H	499	GLU
2	H	503	GLN
2	H	534	HIS
1	I	38	ARG
1	I	42	PRO
1	I	52	LEU
1	I	133	ARG
1	I	165	GLN
2	J	395	THR
2	J	399	MET

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Mol	Chain	Res	Type
2	J	411	LYS
2	J	428	ARG
2	J	497	ASN
2	J	534	HIS
1	K	42	PRO
1	K	52	LEU
1	K	133	ARG
1	K	165	GLN
2	L	364	LEU
2	L	368	ASN
2	L	372	LEU
2	L	411	LYS
2	L	428	ARG
2	L	497	ASN
2	L	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	165	GLN
2	B	361	HIS
2	B	368	ASN
2	B	412	ASN
2	B	497	ASN
2	B	503	GLN
1	C	163	GLN
1	C	165	GLN
2	D	361	HIS
2	D	368	ASN
2	D	412	ASN
2	D	422	ASN
2	D	497	ASN
2	D	503	GLN
1	E	163	GLN
1	E	165	GLN
2	F	361	HIS
2	F	368	ASN
2	F	422	ASN
2	F	497	ASN
1	G	59	ASN
1	G	165	GLN

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Mol	Chain	Res	Type
2	H	361	HIS
2	H	368	ASN
2	H	412	ASN
2	H	422	ASN
2	H	497	ASN
2	H	503	GLN
1	I	165	GLN
2	J	334	GLN
2	J	361	HIS
2	J	368	ASN
2	J	412	ASN
2	J	422	ASN
2	J	497	ASN
2	J	503	GLN
1	K	165	GLN
2	L	361	HIS
2	L	368	ASN
2	L	412	ASN
2	L	422	ASN
2	L	497	ASN
2	L	503	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	CME	B	429	2	8,9,10	0.80	1 (12%)	6,9,11	1.21	1 (16%)
2	CME	D	429	2	8,9,10	0.80	1 (12%)	6,9,11	1.22	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CME	F	429	2	8,9,10	0.85	1 (12%)	6,9,11	1.21	1 (16%)
2	CME	H	429	2	8,9,10	0.83	1 (12%)	6,9,11	1.24	1 (16%)
2	CME	J	429	2	8,9,10	0.82	1 (12%)	6,9,11	1.22	1 (16%)
2	CME	L	429	2	8,9,10	0.85	1 (12%)	6,9,11	1.26	1 (16%)

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
2	CME	B	429	2	-	0/5/8/10	0/0/0/0
2	CME	D	429	2	-	0/5/8/10	0/0/0/0
2	CME	F	429	2	-	0/5/8/10	0/0/0/0
2	CME	H	429	2	-	0/5/8/10	0/0/0/0
2	CME	J	429	2	-	0/5/8/10	0/0/0/0
2	CME	L	429	2	-	0/5/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	429	CME	OH-CZ	-2.05	1.31	1.42
2	F	429	CME	OH-CZ	-2.05	1.31	1.42
2	H	429	CME	OH-CZ	-2.03	1.31	1.42
2	B	429	CME	OH-CZ	-2.02	1.31	1.42
2	D	429	CME	OH-CZ	-2.02	1.31	1.42
2	J	429	CME	OH-CZ	-2.00	1.31	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	429	CME	OH-CZ-CE	2.13	120.17	110.83
2	J	429	CME	OH-CZ-CE	2.21	120.51	110.83
2	H	429	CME	OH-CZ-CE	2.22	120.55	110.83
2	L	429	CME	OH-CZ-CE	2.23	120.59	110.83
2	B	429	CME	OH-CZ-CE	2.24	120.64	110.83
2	D	429	CME	OH-CZ-CE	2.25	120.69	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/200 (100%)	-0.09	11 (5%) 29 27	8, 24, 51, 64	0
1	C	200/200 (100%)	-0.04	14 (7%) 19 18	8, 24, 52, 63	0
1	E	200/200 (100%)	-0.04	9 (4%) 37 36	8, 24, 51, 64	0
1	G	200/200 (100%)	-0.04	13 (6%) 22 21	9, 24, 52, 64	0
1	I	200/200 (100%)	0.08	16 (8%) 15 14	10, 26, 52, 64	0
1	K	200/200 (100%)	0.18	18 (9%) 12 11	11, 27, 52, 64	0
2	B	237/238 (99%)	-0.35	9 (3%) 44 43	9, 16, 42, 65	0
2	D	237/238 (99%)	-0.37	9 (3%) 44 43	9, 16, 42, 64	0
2	F	237/238 (99%)	-0.44	8 (3%) 49 48	9, 16, 42, 64	0
2	H	237/238 (99%)	-0.41	8 (3%) 49 48	9, 16, 42, 65	0
2	J	237/238 (99%)	-0.38	11 (4%) 36 35	11, 19, 43, 65	0
2	L	237/238 (99%)	-0.39	12 (5%) 32 31	10, 18, 44, 64	0
All	All	2622/2628 (99%)	-0.21	138 (5%) 30 29	8, 21, 48, 65	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	99	PHE	7.8
2	B	301	PRO	7.6
2	L	370	GLY	7.3
1	I	101	ALA	7.2
1	K	177	VAL	7.1
2	B	538	CYS	6.5
2	D	369	ASN	6.5
1	K	99	PHE	6.5
1	A	99	PHE	6.3
2	J	370	GLY	6.3
1	C	100	ASP	6.2

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Mol	Chain	Res	Type	RSRZ
2	L	301	PRO	6.0
1	K	178	ASP	5.7
2	D	368	ASN	5.7
2	L	368	ASN	5.7
2	J	368	ASN	5.6
2	B	370	GLY	5.5
1	C	99	PHE	5.5
2	D	301	PRO	5.5
2	H	538	CYS	5.4
2	F	368	ASN	5.4
2	F	301	PRO	5.4
2	J	538	CYS	5.3
2	B	368	ASN	5.2
1	I	99	PHE	5.2
2	L	369	ASN	5.1
1	I	177	VAL	5.1
2	J	369	ASN	5.0
1	K	179	GLY	4.9
1	A	178	ASP	4.9
1	I	100	ASP	4.9
2	H	301	PRO	4.8
2	F	370	GLY	4.8
1	A	101	ALA	4.7
1	G	178	ASP	4.7
1	G	99	PHE	4.6
1	I	178	ASP	4.6
1	K	100	ASP	4.4
2	B	369	ASN	4.4
1	G	177	VAL	4.4
1	G	176	GLU	4.3
2	D	370	GLY	4.3
2	D	538	CYS	4.2
2	L	538	CYS	4.2
1	C	98	THR	4.1
2	F	369	ASN	4.0
1	G	100	ASP	4.0
2	H	414	ARG	4.0
1	E	177	VAL	3.9
2	B	414	ARG	3.8
2	J	537	ASN	3.8
1	I	176	GLU	3.8
2	B	537	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	100	ASP	3.8
1	C	101	ALA	3.8
1	K	176	GLU	3.7
1	I	179	GLY	3.7
2	F	538	CYS	3.7
1	A	100	ASP	3.7
2	J	414	ARG	3.7
1	G	101	ALA	3.7
2	F	414	ARG	3.6
1	E	178	ASP	3.6
1	I	32	ASP	3.4
1	K	180	LYS	3.4
1	K	101	ALA	3.4
1	K	43	ASP	3.4
2	J	301	PRO	3.4
1	E	176	GLU	3.3
1	K	86	GLU	3.3
2	L	305	ASN	3.3
1	A	192	GLU	3.3
1	E	101	ALA	3.2
1	G	179	GLY	3.1
1	G	192	GLU	3.1
2	H	368	ASN	3.1
2	L	537	ASN	3.1
1	C	192	GLU	3.1
1	A	179	GLY	3.1
2	B	305	ASN	3.1
1	G	27	GLY	3.1
1	I	30	THR	3.0
2	L	414	ARG	3.0
2	H	411	LYS	3.0
2	J	433	SER	3.0
1	C	29	PRO	3.0
1	G	24	GLU	3.0
2	D	411	LYS	2.9
1	A	176	GLU	2.9
1	K	42	PRO	2.9
1	I	24	GLU	2.9
2	B	303	GLN	2.9
1	E	179	GLY	2.8
1	K	24	GLU	2.8
1	C	150	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	150	GLN	2.8
2	D	414	ARG	2.8
1	A	177	VAL	2.7
1	K	41	LYS	2.7
2	J	371	GLY	2.6
2	J	411	LYS	2.6
1	K	150	GLN	2.6
2	D	537	ASN	2.6
2	J	412	ASN	2.5
1	A	102	GLY	2.5
2	H	305	ASN	2.4
1	K	149	ALA	2.4
2	L	353	HIS	2.4
1	E	86	GLU	2.4
1	I	29	PRO	2.4
1	C	27	GLY	2.4
1	C	86	GLU	2.4
1	E	150	GLN	2.4
2	L	303	GLN	2.3
2	H	537	ASN	2.3
1	I	27	GLY	2.3
1	K	27	GLY	2.3
2	L	433	SER	2.3
1	C	24	GLU	2.3
1	K	192	GLU	2.3
1	C	32	ASP	2.2
2	L	358	ALA	2.2
1	A	42	PRO	2.2
2	H	353	HIS	2.2
1	I	102	GLY	2.2
1	G	26	ALA	2.2
1	I	192	GLU	2.2
1	A	32	ASP	2.2
1	K	174	ARG	2.2
2	D	305	ASN	2.2
1	G	98	THR	2.2
1	C	179	GLY	2.1
2	F	537	ASN	2.1
1	C	180	LYS	2.1
1	I	98	THR	2.1
2	F	412	ASN	2.0
1	C	41	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	43	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CME	H	429	10/11	0.96	0.11	-	16,18,33,37	0
2	CME	J	429	10/11	0.94	0.10	-	19,21,35,38	0
2	CME	D	429	10/11	0.95	0.11	-	16,18,35,36	0
2	CME	F	429	10/11	0.96	0.11	-	17,18,35,38	0
2	CME	B	429	10/11	0.97	0.11	-	15,18,33,36	0
2	CME	L	429	10/11	0.96	0.09	-	16,21,35,37	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FE	L	600	1/1	0.98	0.04	-5.33	38,38,38,38	0
3	FE	F	600	1/1	0.98	0.03	-5.93	39,39,39,39	0
3	FE	J	600	1/1	0.98	0.03	-7.65	46,46,46,46	0
3	FE	D	600	1/1	0.99	0.02	-	40,40,40,40	0
3	FE	B	600	1/1	0.95	0.04	-	41,41,41,41	0
3	FE	H	600	1/1	0.98	0.06	-	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.