



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:44 PM UTC

PDB ID : 1YKO / pdb_00001yko
Title : Protocatechuate 3,4-Dioxygenase Y408H mutant
Authors : Brown, C.K.; Ohlendorf, D.H.
Deposited on : 2005-01-18
Resolution : 2.54 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

<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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

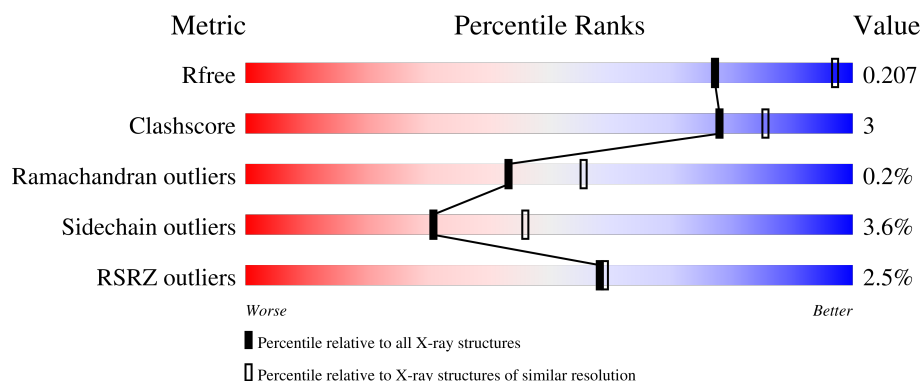
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	3% 88% 10% .
1	C	200	5% 90% 8% .
1	E	200	2% 92% 6% .
1	G	200	4% 90% 8% .
1	I	200	2% 91% 8% .

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Mol	Chain	Length	Quality of chain
1	K	200	2% 92% 6%
2	B	238	3% 86% 13%
2	D	238	2% 87% 11%
2	F	238	3% 88% 10%
2	H	238	% 88% 11%
2	J	238	% 90% 8%
2	L	238	3% 89% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21444 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
			1877	1187	344	337	9			
2	D	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	F	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	H	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	J	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	L	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	TYR	engineered mutation	UNP P00437

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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	CME	CYS	modified residue	UNP P00437
D	408	HIS	TYR	engineered mutation	UNP P00437
D	429	CME	CYS	modified residue	UNP P00437
F	408	HIS	TYR	engineered mutation	UNP P00437
F	429	CME	CYS	modified residue	UNP P00437
H	408	HIS	TYR	engineered mutation	UNP P00437
H	429	CME	CYS	modified residue	UNP P00437
J	408	HIS	TYR	engineered mutation	UNP P00437
J	429	CME	CYS	modified residue	UNP P00437
L	408	HIS	TYR	engineered mutation	UNP P00437
L	429	CME	CYS	modified residue	UNP P00437

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	47	Total O 47 47	0	0
4	B	77	Total O 77 77	0	0
4	C	44	Total O 44 44	0	0
4	D	83	Total O 83 83	0	0
4	E	45	Total O 45 45	0	0
4	F	78	Total O 78 78	0	0

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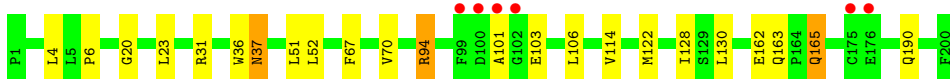
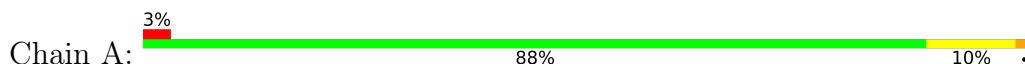
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	45	Total 45	O 45	0	0
4	H	81	Total 81	O 81	0	0
4	I	43	Total 43	O 43	0	0
4	J	83	Total 83	O 83	0	0
4	K	46	Total 46	O 46	0	0
4	L	78	Total 78	O 78	0	0

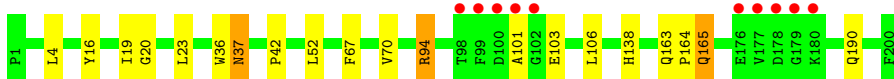
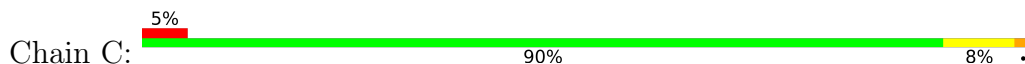
3 Residue-property plots [i](#)

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 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.

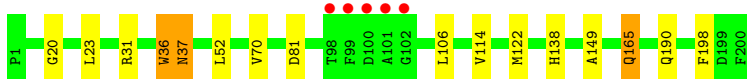
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



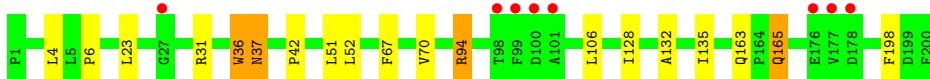
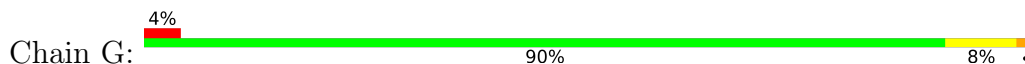
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



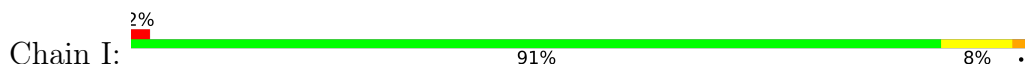
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



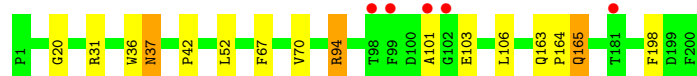
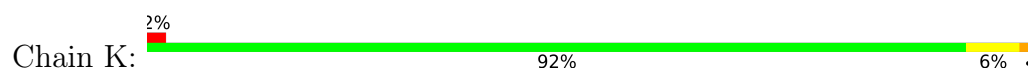
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



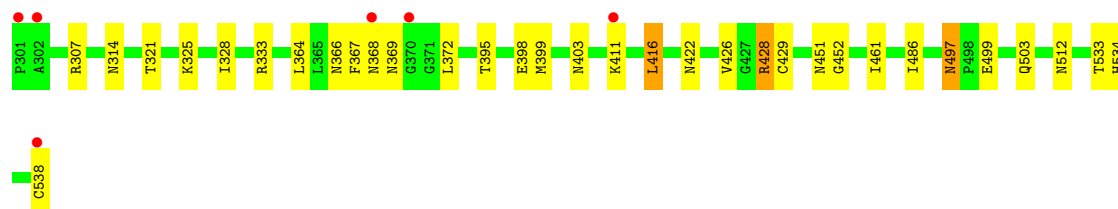
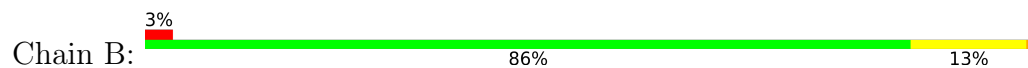
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



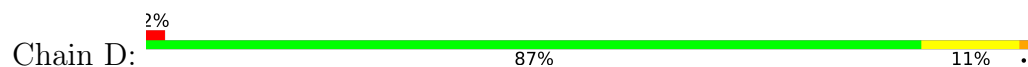
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



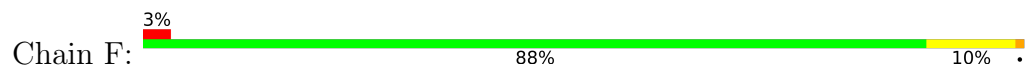
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



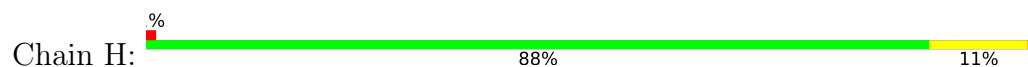
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



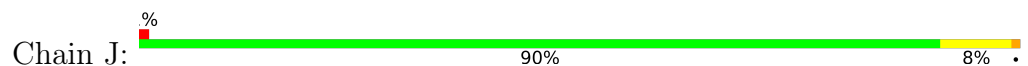
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



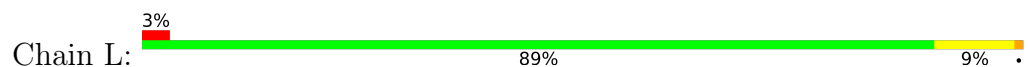
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



- 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	196.59Å 127.63Å 134.45Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	37.27 – 2.54 37.27 – 2.54	Depositor EDS
% Data completeness (in resolution range)	76.1 (37.27-2.54) 76.0 (37.27-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.217 0.178 , 0.207	Depositor DCC
R_{free} test set	1950 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 22.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21444	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.99	6/2195 (0.3%)
1	C	0.62	0/1611	0.99	3/2195 (0.1%)
1	E	0.63	0/1611	1.01	7/2195 (0.3%)
1	G	0.62	0/1611	0.99	6/2195 (0.3%)
1	I	0.65	0/1611	1.00	3/2195 (0.1%)
1	K	0.66	0/1611	0.99	2/2195 (0.1%)
2	B	0.65	1/1922 (0.1%)	1.04	6/2615 (0.2%)
2	D	0.67	1/1922 (0.1%)	1.04	7/2615 (0.3%)
2	F	0.65	1/1922 (0.1%)	1.03	6/2615 (0.2%)
2	H	0.66	1/1922 (0.1%)	1.00	3/2615 (0.1%)
2	J	0.67	1/1922 (0.1%)	1.04	7/2615 (0.3%)
2	L	0.69	1/1922 (0.1%)	1.03	7/2615 (0.3%)
All	All	0.65	6/21198 (0.0%)	1.01	63/28860 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	486	ILE	CA-CB	8.95	1.59	1.54
2	F	486	ILE	CA-CB	7.73	1.58	1.54
2	J	486	ILE	CA-CB	7.66	1.58	1.54
2	L	486	ILE	CA-CB	7.44	1.58	1.54
2	H	486	ILE	CA-CB	7.28	1.58	1.54
2	B	486	ILE	CA-CB	6.31	1.57	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	37	ASN	N-CA-C	9.00	124.09	113.20
1	G	37	ASN	N-CA-C	8.32	123.05	113.15
2	B	325	LYS	N-CA-C	8.21	121.26	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ASN	N-CA-C	8.04	122.72	113.15
2	F	325	LYS	N-CA-C	8.03	121.05	111.33
2	J	325	LYS	N-CA-C	7.80	120.77	111.33
1	E	37	ASN	N-CA-C	7.74	122.36	113.15
1	K	37	ASN	N-CA-C	7.54	122.32	113.20
1	A	37	ASN	N-CA-C	7.45	122.22	113.20
2	L	416	LEU	N-CA-C	6.63	120.83	112.87
1	E	23	LEU	N-CA-C	6.49	118.35	111.28
2	B	366	ASN	N-CA-C	6.48	120.91	113.19
2	H	314	ASN	N-CA-C	-6.46	105.70	113.97
2	D	416	LEU	N-CA-C	6.43	120.59	112.87
2	J	416	LEU	N-CA-C	6.37	120.51	112.87
2	F	366	ASN	N-CA-C	6.10	120.58	113.20
2	D	366	ASN	N-CA-C	6.10	120.33	113.01
2	L	314	ASN	N-CA-C	-6.05	106.23	113.97
2	F	416	LEU	N-CA-C	5.78	119.81	112.87
1	A	23	LEU	N-CA-C	5.76	118.02	111.11
2	L	325	LYS	N-CA-C	5.75	120.86	111.37
1	G	163	GLN	CA-C-N	5.74	125.59	119.28
1	G	163	GLN	C-N-CA	5.74	125.59	119.28
2	B	314	ASN	N-CA-C	-5.68	106.51	113.50
1	E	138	HIS	N-CA-C	5.67	117.62	110.24
1	C	23	LEU	N-CA-C	5.66	118.18	111.33
2	J	366	ASN	N-CA-C	5.64	120.02	113.20
1	A	163	GLN	CA-C-N	5.63	125.74	119.32
1	A	163	GLN	C-N-CA	5.63	125.74	119.32
2	B	367	PHE	N-CA-C	-5.62	105.46	112.93
2	F	314	ASN	N-CA-C	-5.62	106.59	113.50
2	H	366	ASN	N-CA-C	5.59	119.72	113.01
1	G	36	TRP	N-CA-C	5.58	118.97	108.65
1	I	23	LEU	N-CA-C	5.54	118.04	111.33
2	J	367	PHE	N-CA-C	-5.48	105.71	112.72
2	D	325	LYS	N-CA-C	5.46	120.38	111.37
2	H	371	GLY	N-CA-C	5.45	118.48	110.80
2	D	371	GLY	N-CA-C	5.42	118.50	110.42
2	L	321	THR	CA-C-N	5.37	126.55	119.84
2	L	321	THR	C-N-CA	5.37	126.55	119.84
1	E	149	ALA	N-CA-C	5.36	117.81	111.33
2	J	460	HIS	N-CA-C	5.34	117.18	109.07
1	G	23	LEU	N-CA-C	5.31	117.75	111.33
1	K	198	PHE	N-CA-C	5.27	118.59	110.42
2	J	314	ASN	N-CA-C	-5.27	107.02	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	366	ASN	N-CA-C	5.27	119.55	113.18
1	A	162	GLU	N-CA-C	5.25	117.42	111.11
1	C	138	HIS	N-CA-C	5.25	117.07	110.24
1	E	81	ASP	N-CA-C	5.22	117.06	111.36
2	F	321	THR	CA-C-N	5.21	126.36	119.84
2	F	321	THR	C-N-CA	5.21	126.36	119.84
2	B	321	THR	CA-C-N	5.21	126.35	119.84
2	B	321	THR	C-N-CA	5.21	126.35	119.84
2	D	469	SER	N-CA-C	5.18	116.16	108.86
2	D	321	THR	CA-C-N	5.13	126.25	119.84
2	D	321	THR	C-N-CA	5.13	126.25	119.84
1	E	36	TRP	N-CA-C	5.10	118.08	108.65
1	E	198	PHE	N-CA-C	5.09	118.03	110.14
2	J	371	GLY	N-CA-C	5.09	118.00	110.42
1	I	81	ASP	N-CA-C	5.08	117.71	111.82
1	A	130	LEU	N-CA-C	5.07	116.79	108.52
2	L	451	ASN	N-CA-C	-5.06	100.02	110.80
1	G	198	PHE	N-CA-C	5.03	118.22	110.42

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	14	0
1	C	1571	0	1499	10	0
1	E	1571	0	1499	7	0
1	G	1571	0	1499	12	0
1	I	1571	0	1499	9	0
1	K	1571	0	1499	9	0
2	B	1877	0	1821	14	0
2	D	1877	0	1821	14	0
2	F	1877	0	1821	13	0
2	H	1877	0	1821	14	0
2	J	1877	0	1821	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1877	0	1821	10	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	47	0	0	0	0
4	B	77	0	0	1	0
4	C	44	0	0	0	0
4	D	83	0	0	1	0
4	E	45	0	0	0	0
4	F	78	0	0	1	0
4	G	45	0	0	0	0
4	H	81	0	0	0	0
4	I	43	0	0	0	0
4	J	83	0	0	0	0
4	K	46	0	0	0	0
4	L	78	0	0	0	0
All	All	21444	0	19920	112	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 3.

All (112) 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:C:165:GLN:HE21	1:C:165:GLN:H	1.29	0.81
1:I:165:GLN:H	1:I:165:GLN:HE21	1.41	0.66
2:B:497:ASN:HD22	2:B:499:GLU:H	1.45	0.62
2:F:497:ASN:HD22	2:F:499:GLU:H	1.48	0.60
2:L:497:ASN:HD22	2:L:499:GLU:H	1.49	0.59
2:H:369:ASN:H	2:H:422:ASN:HD22	1.50	0.59
1:I:165:GLN:H	1:I:165:GLN:NE2	2.00	0.59
1:E:165:GLN:NE2	1:E:165:GLN:H	2.01	0.59
1:K:165:GLN:NE2	1:K:165:GLN:H	2.01	0.59
2:H:497:ASN:HD22	2:H:499:GLU:H	1.51	0.58
2:B:307:ARG:HG2	2:B:533:THR:HG22	1.86	0.58
2:D:307:ARG:HG2	2:D:533:THR:HG22	1.86	0.57
1:C:165:GLN:H	1:C:165:GLN:NE2	2.01	0.57
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ARG:NH1	2:F:428:ARG:HG2	2.20	0.57
1:K:20:GLY:HA2	2:L:426:VAL:HG13	1.87	0.57
1:I:51:LEU:HD12	1:I:106:LEU:HD23	1.87	0.56
1:A:6:PRO:HB2	2:B:503:GLN:HE22	1.70	0.56
2:J:497:ASN:HD22	2:J:499:GLU:H	1.53	0.55
2:D:368:ASN:ND2	2:D:371:GLY:H	2.05	0.53
1:G:6:PRO:HB2	2:H:503:GLN:HE22	1.74	0.53
2:J:416:LEU:H	2:J:416:LEU:HD23	1.74	0.53
1:G:165:GLN:NE2	1:G:165:GLN:H	2.05	0.53
1:I:67:PHE:HZ	1:I:94:ARG:HD2	1.74	0.52
1:I:20:GLY:HA2	2:J:426:VAL:HG13	1.90	0.52
2:D:416:LEU:H	2:D:416:LEU:HD23	1.74	0.52
2:F:416:LEU:H	2:F:416:LEU:HD23	1.75	0.52
1:K:67:PHE:HZ	1:K:94:ARG:HD2	1.74	0.52
1:A:165:GLN:NE2	1:A:165:GLN:H	2.07	0.51
2:D:369:ASN:H	2:D:422:ASN:HD22	1.59	0.51
1:G:31:ARG:NH1	2:H:428:ARG:HG2	2.25	0.50
2:H:335:ALA:HB2	2:L:328:ILE:HD12	1.94	0.50
2:L:307:ARG:HG2	2:L:533:THR:HG22	1.92	0.50
1:G:36:TRP:CG	1:G:37:ASN:H	2.29	0.50
1:A:20:GLY:HA2	2:B:426:VAL:HG13	1.94	0.50
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.77	0.50
2:L:416:LEU:H	2:L:416:LEU:HD23	1.76	0.49
1:C:36:TRP:CG	1:C:37:ASN:H	2.30	0.49
2:B:369:ASN:H	2:B:422:ASN:HD22	1.58	0.49
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.78	0.49
2:B:416:LEU:H	2:B:416:LEU:HD23	1.77	0.49
1:C:20:GLY:HA2	2:D:426:VAL:HG13	1.94	0.49
1:A:36:TRP:CG	1:A:37:ASN:H	2.31	0.49
2:B:328:ILE:HD12	2:D:335:ALA:HB2	1.95	0.48
2:H:369:ASN:H	2:H:422:ASN:ND2	2.12	0.48
2:B:497:ASN:ND2	2:B:499:GLU:H	2.11	0.48
1:E:190:GLN:HG3	2:F:333:ARG:HG2	1.96	0.48
1:E:20:GLY:HA2	2:F:426:VAL:HG13	1.96	0.47
2:H:307:ARG:HG2	2:H:533:THR:HG22	1.95	0.47
1:K:36:TRP:CG	1:K:37:ASN:H	2.31	0.47
1:G:165:GLN:H	1:G:165:GLN:HE21	1.63	0.47
1:K:67:PHE:CZ	1:K:94:ARG:HD2	2.48	0.47
1:G:67:PHE:HZ	1:G:94:ARG:HD2	1.78	0.46
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.98	0.46
1:E:36:TRP:CG	1:E:37:ASN:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:HG21	1:E:106:LEU:HD21	1.98	0.45
2:J:307:ARG:HG2	2:J:533:THR:HG22	1.98	0.45
2:F:307:ARG:HG2	2:F:533:THR:HG22	1.99	0.45
2:F:497:ASN:ND2	2:F:499:GLU:H	2.14	0.45
2:F:403:ASN:HB2	4:F:2620:HOH:O	2.15	0.44
2:D:320:LEU:HD13	2:D:333:ARG:HH12	1.81	0.44
1:G:51:LEU:HD12	1:G:106:LEU:HD23	1.98	0.44
1:G:132:ALA:HB3	1:G:135:ILE:HD12	1.99	0.44
1:I:36:TRP:CG	1:I:37:ASN:H	2.36	0.44
1:K:31:ARG:NH1	2:L:428:ARG:HG2	2.33	0.44
1:K:70:VAL:HG21	1:K:106:LEU:HD21	2.00	0.44
1:I:70:VAL:HG12	1:I:128:ILE:HG12	2.00	0.44
1:A:70:VAL:HG12	1:A:128:ILE:HG12	2.00	0.44
2:F:361:HIS:H	2:F:361:HIS:CD2	2.36	0.43
1:A:31:ARG:NH1	2:B:428:ARG:HG2	2.34	0.43
1:C:190:GLN:HG3	2:D:333:ARG:HG2	2.01	0.43
2:H:489:CYS:HA	2:H:490:PRO:HD3	1.92	0.43
1:I:16:TYR:O	1:I:19:ILE:HG12	2.18	0.43
1:C:16:TYR:O	1:C:19:ILE:HG12	2.17	0.43
2:F:369:ASN:H	2:F:422:ASN:HD22	1.66	0.43
2:H:416:LEU:H	2:H:416:LEU:HD23	1.83	0.43
2:B:403:ASN:HB2	4:B:620:HOH:O	2.19	0.43
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.54	0.43
1:G:6:PRO:HB2	2:H:503:GLN:NE2	2.34	0.43
1:C:101:ALA:C	1:C:103:GLU:H	2.26	0.43
2:L:497:ASN:ND2	2:L:499:GLU:H	2.15	0.43
2:L:315:TRP:HZ2	2:L:503:GLN:HE21	1.66	0.42
2:H:359:HIS:O	2:H:366:ASN:HB3	2.19	0.42
1:G:67:PHE:CZ	1:G:94:ARG:HD2	2.54	0.42
2:J:368:ASN:ND2	2:J:371:GLY:H	2.16	0.42
1:K:101:ALA:C	1:K:103:GLU:H	2.28	0.42
1:K:163:GLN:HA	1:K:164:PRO:HD3	1.91	0.42
1:A:101:ALA:C	1:A:103:GLU:H	2.28	0.42
2:D:497:ASN:ND2	2:D:499:GLU:H	2.18	0.41
2:H:320:LEU:HD13	2:H:333:ARG:HH22	1.85	0.41
1:C:163:GLN:HA	1:C:164:PRO:HD3	1.92	0.41
1:G:70:VAL:HG21	1:G:106:LEU:HD21	2.01	0.41
2:D:361:HIS:CD2	2:D:361:HIS:H	2.37	0.41
2:F:348:GLY:HA3	2:F:469:SER:HA	2.01	0.41
2:H:361:HIS:CD2	2:H:361:HIS:H	2.38	0.41
2:D:497:ASN:HD22	2:D:498:PRO:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:403:ASN:HB2	4:D:1620:HOH:O	2.20	0.41
1:C:70:VAL:HG21	1:C:106:LEU:HD21	2.01	0.41
2:L:361:HIS:CD2	2:L:361:HIS:H	2.39	0.41
2:L:382:GLY:HA2	2:L:522:ARG:HE	1.85	0.41
1:A:190:GLN:HG3	2:B:333:ARG:HG2	2.01	0.41
2:B:399:MET:HE2	2:B:461:ILE:HG21	2.02	0.41
2:B:451:ASN:HB3	2:B:452:GLY:H	1.76	0.41
1:G:70:VAL:HG12	1:G:128:ILE:HG12	2.02	0.41
2:F:333:ARG:HE	2:F:333:ARG:HA	1.86	0.40
1:A:94:ARG:HH22	2:B:398:GLU:CD	2.28	0.40
2:D:451:ASN:HB3	2:D:452:GLY:H	1.71	0.40
1:A:51:LEU:HD12	1:A:106:LEU:HD23	2.03	0.40
1:I:132:ALA:HB3	1:I:135:ILE:HD12	2.03	0.40
2:D:328:ILE:HD12	2:F:335:ALA:HB2	2.03	0.40
1:E:114:VAL:HG23	1:E:122:MET:HE3	2.04	0.40
2:H:328:ILE:HD12	2:J:335:ALA:HB2	2.03	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%)	194 (98%)	4 (2%)	0	100	100
1	C	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	E	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	G	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	I	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	K	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
2	B	235/238 (99%)	227 (97%)	7 (3%)	1 (0%)	30	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	235/238 (99%)	229 (97%)	5 (2%)	1 (0%)	30	39
2	F	235/238 (99%)	228 (97%)	6 (3%)	1 (0%)	30	39
2	H	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	30	39
2	J	235/238 (99%)	230 (98%)	4 (2%)	1 (0%)	30	39
2	L	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	30	39
All	All	2598/2628 (99%)	2519 (97%)	73 (3%)	6 (0%)	43	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	368	ASN
2	D	368	ASN
2	F	368	ASN
2	H	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%)	158 (98%)	4 (2%)	42	60
1	C	162/163 (99%)	157 (97%)	5 (3%)	35	53
1	E	162/163 (99%)	160 (99%)	2 (1%)	63	78
1	G	162/163 (99%)	157 (97%)	5 (3%)	35	53
1	I	162/163 (99%)	158 (98%)	4 (2%)	42	60
1	K	162/163 (99%)	158 (98%)	4 (2%)	42	60
2	B	199/201 (99%)	189 (95%)	10 (5%)	22	33
2	D	199/201 (99%)	191 (96%)	8 (4%)	28	42
2	F	199/201 (99%)	189 (95%)	10 (5%)	22	33
2	H	199/201 (99%)	191 (96%)	8 (4%)	28	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	199/201 (99%)	189 (95%)	10 (5%)	22	33
2	L	199/201 (99%)	190 (96%)	9 (4%)	24	38
All	All	2166/2184 (99%)	2087 (96%)	79 (4%)	31	46

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	52	LEU
1	A	94	ARG
1	A	165	GLN
2	B	364	LEU
2	B	372	LEU
2	B	395	THR
2	B	411	LYS
2	B	416	LEU
2	B	428	ARG
2	B	497	ASN
2	B	512	ASN
2	B	534	HIS
2	B	538	CYS
1	C	4	LEU
1	C	42	PRO
1	C	52	LEU
1	C	94	ARG
1	C	165	GLN
2	D	333	ARG
2	D	364	LEU
2	D	372	LEU
2	D	395	THR
2	D	411	LYS
2	D	416	LEU
2	D	428	ARG
2	D	478	LEU
1	E	52	LEU
1	E	165	GLN
2	F	333	ARG
2	F	372	LEU
2	F	395	THR
2	F	411	LYS
2	F	416	LEU

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Mol	Chain	Res	Type
2	F	428	ARG
2	F	478	LEU
2	F	497	ASN
2	F	534	HIS
2	F	538	CYS
1	G	4	LEU
1	G	42	PRO
1	G	52	LEU
1	G	94	ARG
1	G	165	GLN
2	H	364	LEU
2	H	372	LEU
2	H	395	THR
2	H	411	LYS
2	H	428	ARG
2	H	478	LEU
2	H	497	ASN
2	H	534	HIS
1	I	42	PRO
1	I	52	LEU
1	I	94	ARG
1	I	165	GLN
2	J	364	LEU
2	J	395	THR
2	J	399	MET
2	J	411	LYS
2	J	416	LEU
2	J	428	ARG
2	J	478	LEU
2	J	497	ASN
2	J	534	HIS
2	J	538	CYS
1	K	42	PRO
1	K	52	LEU
1	K	94	ARG
1	K	165	GLN
2	L	364	LEU
2	L	372	LEU
2	L	395	THR
2	L	411	LYS
2	L	416	LEU
2	L	426	VAL

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Mol	Chain	Res	Type
2	L	428	ARG
2	L	497	ASN
2	L	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	59	ASN
1	A	90	ASN
1	A	115	ASN
1	A	163	GLN
1	A	165	GLN
2	B	305	ASN
2	B	350	ASN
2	B	361	HIS
2	B	412	ASN
2	B	422	ASN
2	B	497	ASN
2	B	503	GLN
2	B	530	GLN
2	B	537	ASN
1	C	11	GLN
1	C	59	ASN
1	C	140	HIS
1	C	163	GLN
1	C	165	GLN
2	D	314	ASN
2	D	334	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
2	D	537	ASN
1	E	90	ASN
1	E	115	ASN
1	E	163	GLN
1	E	165	GLN
2	F	334	GLN
2	F	361	HIS

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Mol	Chain	Res	Type
2	F	412	ASN
2	F	422	ASN
2	F	497	ASN
2	F	503	GLN
2	F	511	ASN
1	G	59	ASN
1	G	116	ASN
1	G	163	GLN
1	G	165	GLN
2	H	305	ASN
2	H	314	ASN
2	H	334	GLN
2	H	350	ASN
2	H	361	HIS
2	H	412	ASN
2	H	422	ASN
2	H	497	ASN
2	H	503	GLN
2	H	511	ASN
2	H	537	ASN
1	I	163	GLN
1	I	165	GLN
2	J	314	ASN
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	512	ASN
1	K	59	ASN
1	K	90	ASN
1	K	140	HIS
1	K	163	GLN
1	K	165	GLN
2	L	350	ASN
2	L	361	HIS
2	L	412	ASN
2	L	497	ASN
2	L	503	GLN
2	L	537	ASN

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	H	429	2	8,9,10	0.95	1 (12%)	6,9,11	1.33	1 (16%)
2	CME	B	429	2	8,9,10	0.97	1 (12%)	6,9,11	1.29	1 (16%)
2	CME	F	429	2	8,9,10	1.00	1 (12%)	6,9,11	1.08	1 (16%)
2	CME	D	429	2	8,9,10	0.93	1 (12%)	6,9,11	1.14	1 (16%)
2	CME	J	429	2	8,9,10	0.99	1 (12%)	6,9,11	1.31	1 (16%)
2	CME	L	429	2	8,9,10	0.95	1 (12%)	6,9,11	1.22	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	H	429	2	-	1/5/8/10	-
2	CME	B	429	2	-	1/5/8/10	-
2	CME	F	429	2	-	1/5/8/10	-
2	CME	D	429	2	-	0/5/8/10	-
2	CME	J	429	2	-	1/5/8/10	-
2	CME	L	429	2	-	2/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	429	CME	OH-CZ	-2.35	1.30	1.42
2	D	429	CME	OH-CZ	-2.35	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	429	CME	OH-CZ	-2.35	1.30	1.42
2	L	429	CME	OH-CZ	-2.34	1.30	1.42
2	F	429	CME	OH-CZ	-2.33	1.30	1.42
2	H	429	CME	OH-CZ	-2.27	1.30	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	429	CME	OH-CZ-CE	2.84	121.92	110.82
2	B	429	CME	OH-CZ-CE	2.79	121.71	110.82
2	H	429	CME	OH-CZ-CE	2.75	121.57	110.82
2	L	429	CME	OH-CZ-CE	2.69	121.34	110.82
2	D	429	CME	OH-CZ-CE	2.57	120.87	110.82
2	F	429	CME	OH-CZ-CE	2.45	120.37	110.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	429	CME	CZ-CE-SD-SG
2	B	429	CME	SD-CE-CZ-OH
2	H	429	CME	SD-CE-CZ-OH
2	J	429	CME	SD-CE-CZ-OH
2	L	429	CME	SD-CE-CZ-OH
2	F	429	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

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

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%)	0.04	6 (3%) 52 54	8, 27, 54, 72	0
1	C	200/200 (100%)	0.14	10 (5%) 34 33	8, 28, 54, 71	0
1	E	200/200 (100%)	0.07	5 (2%) 58 59	8, 28, 54, 72	0
1	G	200/200 (100%)	0.05	8 (4%) 42 43	9, 28, 54, 73	0
1	I	200/200 (100%)	0.08	3 (1%) 72 73	10, 30, 55, 73	0
1	K	200/200 (100%)	0.20	5 (2%) 58 59	11, 31, 55, 73	0
2	B	237/238 (99%)	-0.27	6 (2%) 58 59	9, 19, 51, 71	0
2	D	237/238 (99%)	-0.22	4 (1%) 69 69	8, 19, 51, 71	0
2	F	237/238 (99%)	-0.22	6 (2%) 58 59	9, 20, 52, 69	0
2	H	237/238 (99%)	-0.22	3 (1%) 75 75	9, 19, 51, 69	0
2	J	237/238 (99%)	-0.19	3 (1%) 75 75	10, 21, 52, 70	0
2	L	237/238 (99%)	-0.11	6 (2%) 58 59	11, 21, 52, 71	0
All	All	2622/2628 (99%)	-0.07	65 (2%) 58 59	8, 24, 54, 73	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	THR	5.1
1	C	99	PHE	4.4
2	F	538	CYS	3.9
1	C	101	ALA	3.7
1	G	99	PHE	3.7
1	G	100	ASP	3.7
1	K	98	THR	3.7
1	C	179	GLY	3.5
1	K	102	GLY	3.5
1	K	99	PHE	3.4
1	C	180	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	99	PHE	3.4
1	A	176	GLU	3.3
1	G	101	ALA	3.3
1	C	100	ASP	3.3
1	I	99	PHE	3.2
2	D	538	CYS	3.2
1	E	101	ALA	3.2
2	L	368	ASN	3.1
2	H	538	CYS	3.0
2	F	370	GLY	2.9
2	L	370	GLY	2.9
1	G	98	THR	2.9
1	A	101	ALA	2.9
2	B	370	GLY	2.9
1	I	101	ALA	2.8
2	H	303	GLN	2.8
2	B	301	PRO	2.8
1	E	99	PHE	2.8
2	F	414	ARG	2.7
1	E	98	THR	2.7
2	J	538	CYS	2.6
2	B	368	ASN	2.5
1	C	102	GLY	2.5
1	E	102	GLY	2.5
1	E	100	ASP	2.5
2	L	303	GLN	2.4
2	L	537	ASN	2.4
1	A	102	GLY	2.4
1	A	175	CYS	2.4
1	K	181	THR	2.3
1	G	27	GLY	2.3
2	D	370	GLY	2.3
1	G	177	VAL	2.3
2	F	368	ASN	2.3
1	K	101	ALA	2.3
2	H	414	ARG	2.2
1	C	178	ASP	2.2
2	F	303	GLN	2.2
1	G	178	ASP	2.2
1	G	176	GLU	2.2
2	D	368	ASN	2.2
2	L	538	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	176	GLU	2.1
2	L	301	PRO	2.1
1	I	27	GLY	2.1
2	B	302	ALA	2.1
2	J	369	ASN	2.1
2	D	301	PRO	2.1
2	B	411	LYS	2.0
2	F	301	PRO	2.0
2	B	538	CYS	2.0
1	C	177	VAL	2.0
2	J	368	ASN	2.0
1	A	100	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. 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	B-factors(Å ²)	Q<0.9
2	CME	J	429	10/11	0.94	0.09	23,25,37,39	0
2	CME	D	429	10/11	0.96	0.08	19,24,36,38	0
2	CME	F	429	10/11	0.97	0.08	19,22,37,41	0
2	CME	H	429	10/11	0.97	0.08	19,22,36,38	0
2	CME	B	429	10/11	0.97	0.07	18,22,35,37	0
2	CME	L	429	10/11	0.97	0.06	22,25,37,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	FE	H	600	1/1	0.97	0.04	40,40,40,40	0
3	FE	L	600	1/1	0.97	0.04	37,37,37,37	0
3	FE	F	600	1/1	0.98	0.03	42,42,42,42	0
3	FE	B	600	1/1	0.98	0.03	41,41,41,41	0
3	FE	J	600	1/1	0.98	0.03	51,51,51,51	0
3	FE	D	600	1/1	0.98	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.