



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:29 AM UTC

PDB ID : 3E3I / pdb_00003e3i
Title : H. influenzae beta-carbonic anhydrase, variant G41A with 100 mM bicarbonate
Authors : Rowlett, R.S.; Failing, H.
Deposited on : 2008-08-07
Resolution : 2.00 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:

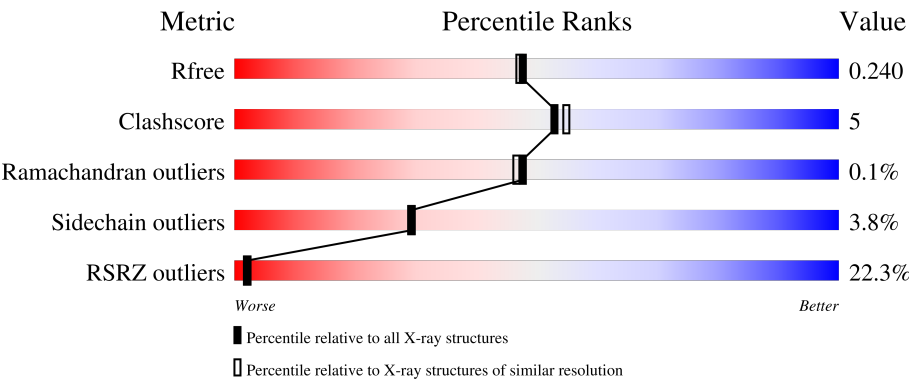
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	229	10% 76% 14% • 9%
1	B	229	10% 81% 10% • 7%
1	C	229	11% 78% 11% • 9%
1	D	229	14% 83% 9% • 7%
1	E	229	16% 80% 11% • 7%

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Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	
1	I	229	
1	J	229	
1	K	229	
1	L	229	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCT	B	233	-	-	X	-
4	BCT	C	232	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21039 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 Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	2	0
			1683	1069	300	305	9			
1	B	212	Total	C	N	O	S	0	1	0
			1711	1087	304	311	9			
1	C	208	Total	C	N	O	S	0	1	0
			1681	1067	300	305	9			
1	D	213	Total	C	N	O	S	0	1	0
			1722	1094	306	313	9			
1	E	212	Total	C	N	O	S	0	1	0
			1714	1088	305	312	9			
1	F	208	Total	C	N	O	S	0	1	0
			1680	1070	300	301	9			
1	G	214	Total	C	N	O	S	0	0	0
			1716	1090	305	312	9			
1	H	209	Total	C	N	O	S	0	1	0
			1693	1075	302	307	9			
1	I	210	Total	C	N	O	S	0	1	0
			1696	1078	302	307	9			
1	J	205	Total	C	N	O	S	0	2	0
			1669	1063	300	297	9			
1	K	209	Total	C	N	O	S	0	1	0
			1693	1075	302	307	9			
1	L	206	Total	C	N	O	S	0	0	0
			1656	1052	297	298	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	GLY	engineered mutation	UNP P45148
B	41	ALA	GLY	engineered mutation	UNP P45148
C	41	ALA	GLY	engineered mutation	UNP P45148
D	41	ALA	GLY	engineered mutation	UNP P45148
E	41	ALA	GLY	engineered mutation	UNP P45148

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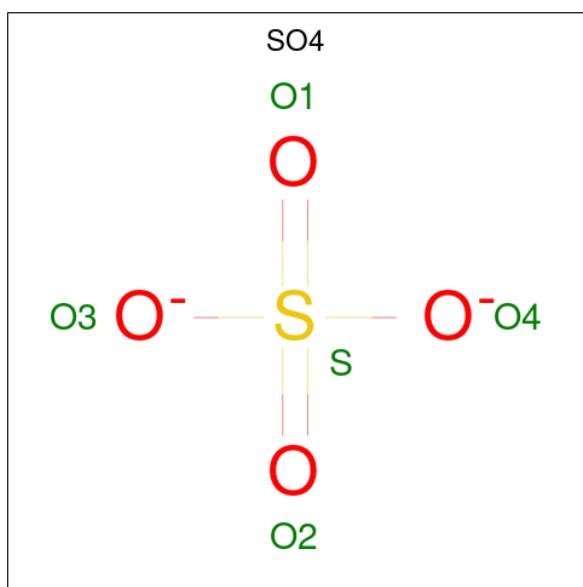
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Chain	Residue	Modelled	Actual	Comment	Reference
F	41	ALA	GLY	engineered mutation	UNP P45148
G	41	ALA	GLY	engineered mutation	UNP P45148
H	41	ALA	GLY	engineered mutation	UNP P45148
I	41	ALA	GLY	engineered mutation	UNP P45148
J	41	ALA	GLY	engineered mutation	UNP P45148
K	41	ALA	GLY	engineered mutation	UNP P45148
L	41	ALA	GLY	engineered mutation	UNP P45148

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

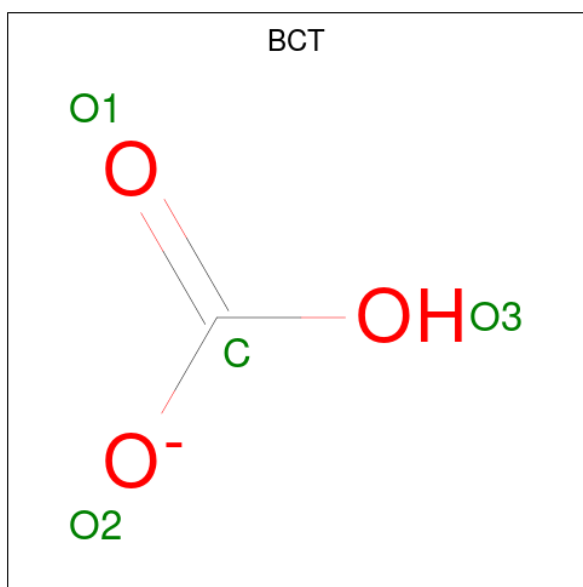
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	1	3		
4	C	1	Total	C	O	0	0
			4	1	3		
4	D	1	Total	C	O	0	0
			4	1	3		
4	E	1	Total	C	O	0	0
			4	1	3		
4	F	1	Total	C	O	0	0
			4	1	3		
4	G	1	Total	C	O	0	0
			4	1	3		
4	H	1	Total	C	O	0	0
			4	1	3		
4	I	1	Total	C	O	0	0
			4	1	3		
4	J	1	Total	C	O	0	0
			4	1	3		
4	K	1	Total	C	O	0	0
			4	1	3		
4	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		

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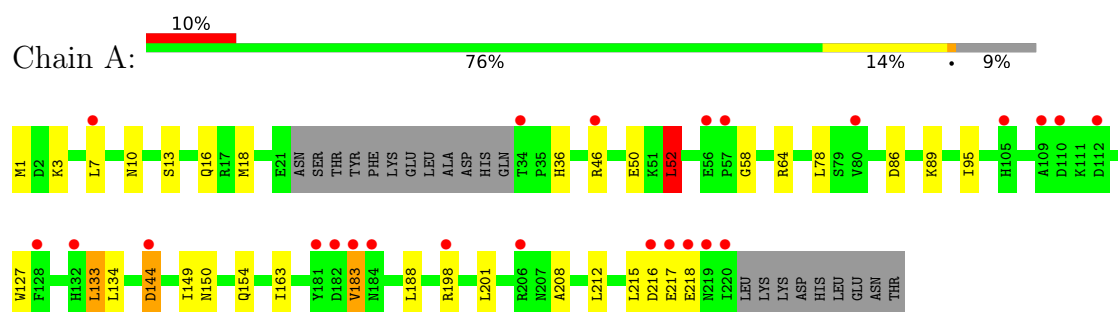
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	59	Total 59	O 59	0	0
5	C	43	Total 43	O 43	0	0
5	D	53	Total 53	O 53	0	0
5	E	65	Total 65	O 65	0	0
5	F	56	Total 56	O 56	0	0
5	G	54	Total 54	O 54	0	0
5	H	50	Total 50	O 50	0	0
5	I	46	Total 46	O 46	0	0
5	J	43	Total 43	O 43	0	0
5	K	44	Total 44	O 44	0	0
5	L	42	Total 42	O 42	0	0

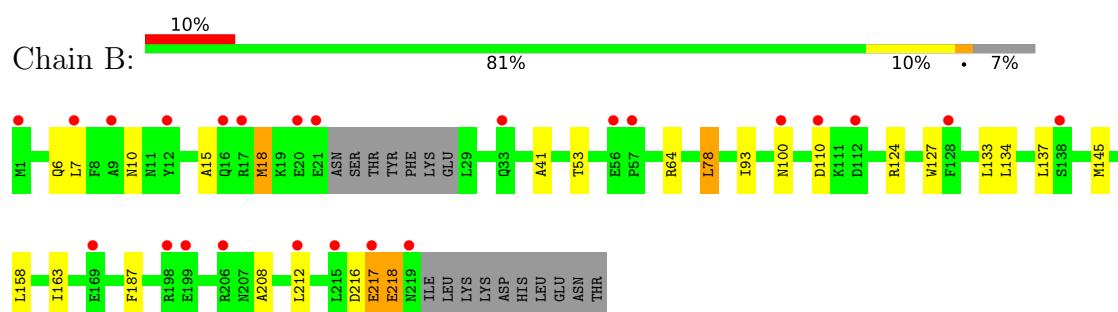
3 Residue-property plots [i](#)

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.

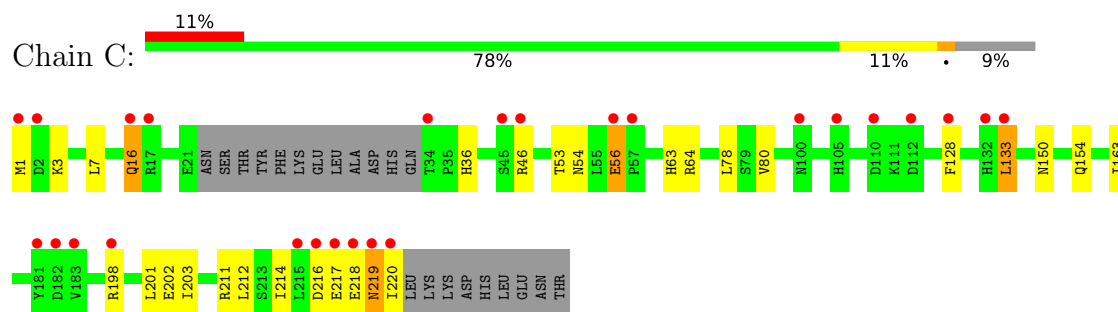
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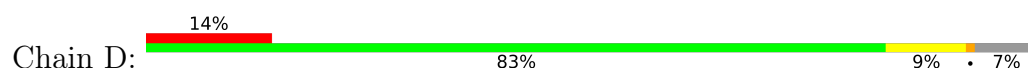
• Molecule 1: Carbonic anhydrase 2

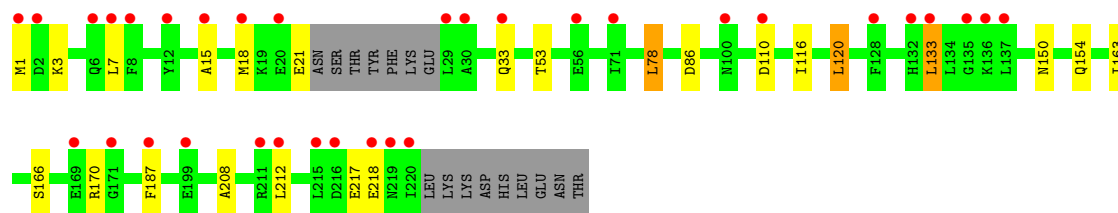


• Molecule 1: Carbonic anhydrase 2

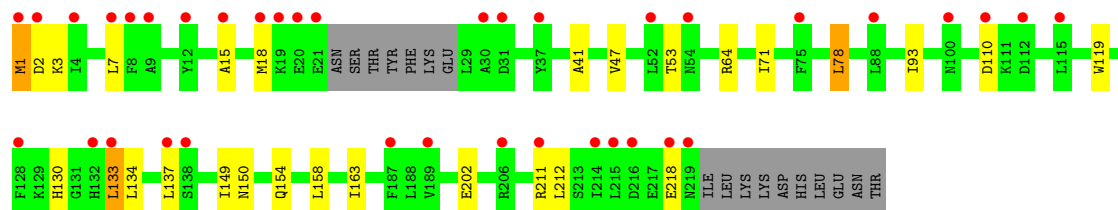
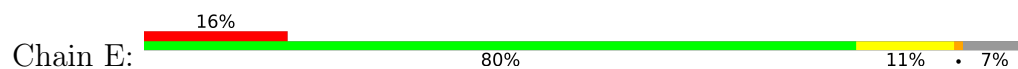


• Molecule 1: Carbonic anhydrase 2

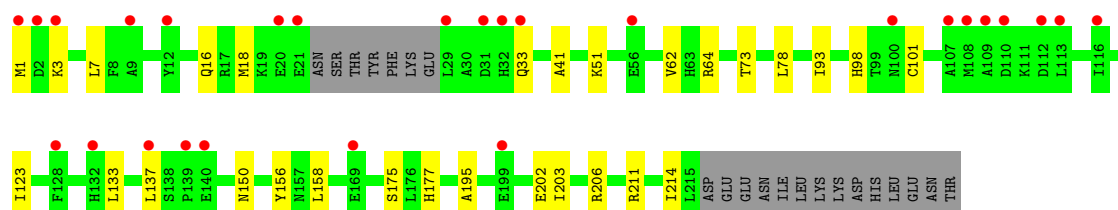
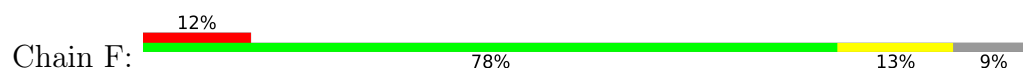




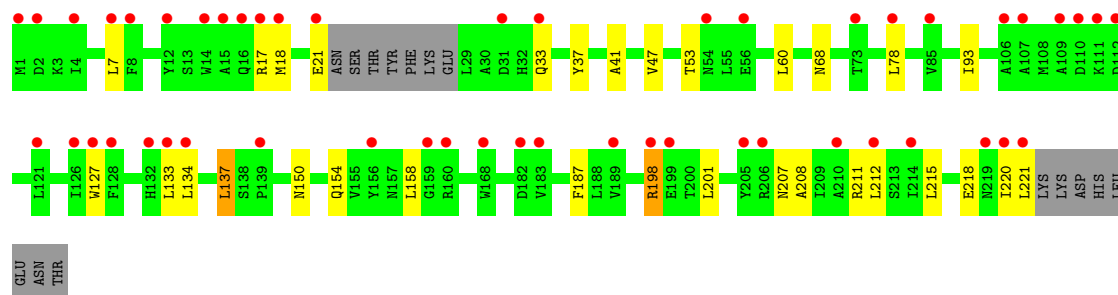
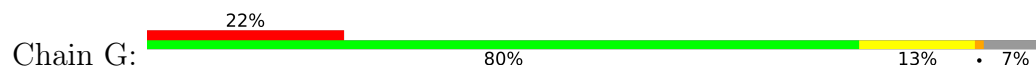
• Molecule 1: Carbonic anhydrase 2



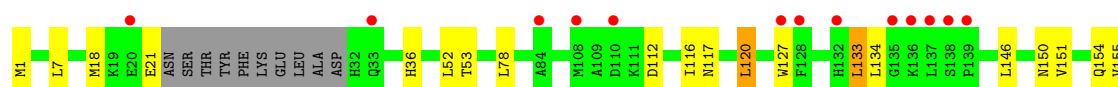
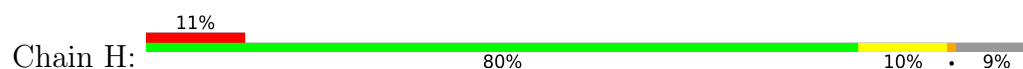
• Molecule 1: Carbonic anhydrase 2

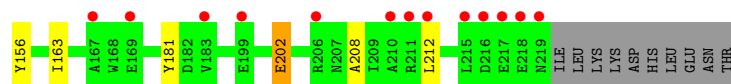


• Molecule 1: Carbonic anhydrase 2

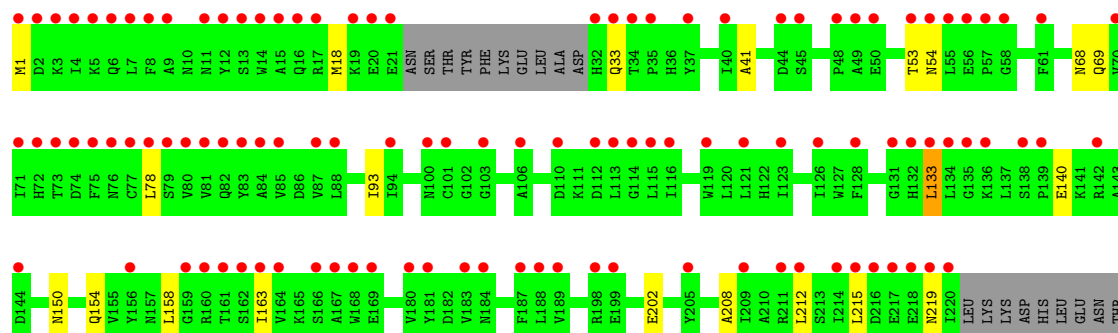
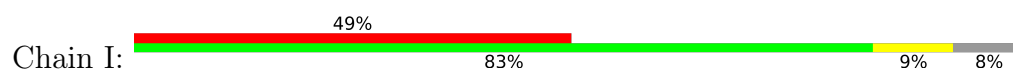


• Molecule 1: Carbonic anhydrase 2

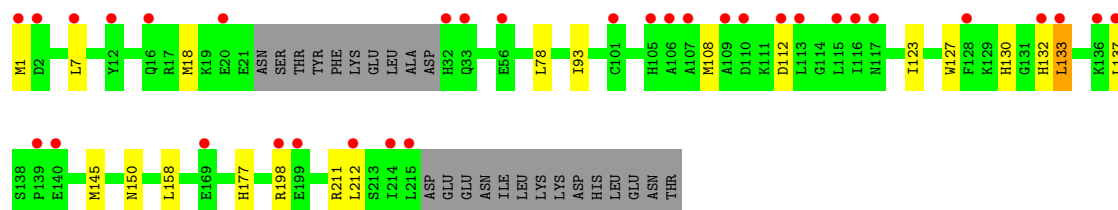
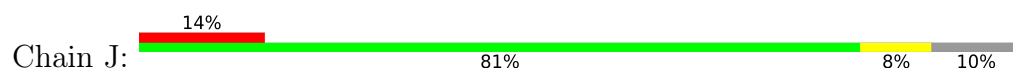




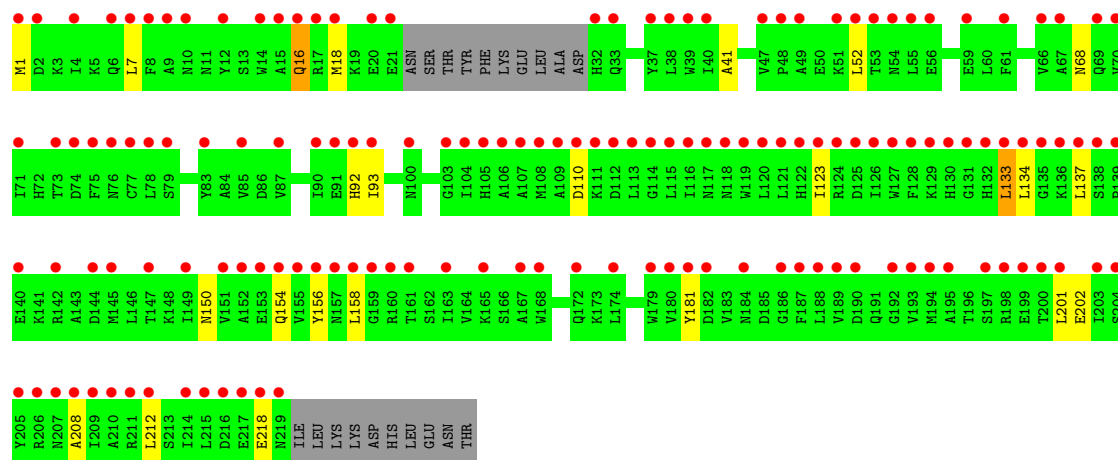
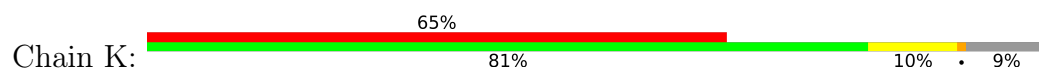
- Molecule 1: Carbonic anhydrase 2



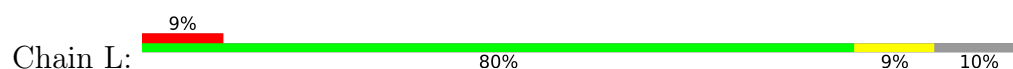
- Molecule 1: Carbonic anhydrase 2

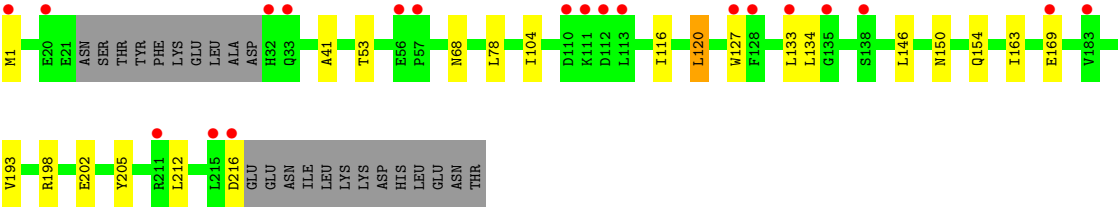


- Molecule 1: Carbonic anhydrase 2



- Molecule 1: Carbonic anhydrase 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.59Å 144.44Å 104.89Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	29.75 – 2.00 29.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (29.75-2.00) 89.5 (29.75-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.236 0.207 , 0.240	Depositor DCC
R_{free} test set	10347 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtrriage
Anisotropy	0.043	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21039	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9966e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BCT, SO4, ZN

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	0.67	0/1725	0.84	1/2336 (0.0%)
1	B	0.64	0/1751	0.79	0/2371
1	C	0.66	0/1717	0.84	0/2325
1	D	0.64	0/1759	0.78	0/2382
1	E	0.69	0/1751	0.83	1/2371 (0.0%)
1	F	0.65	0/1717	0.81	1/2325 (0.0%)
1	G	0.68	0/1752	0.80	0/2373
1	H	0.66	0/1730	0.80	0/2342
1	I	0.64	0/1733	0.76	0/2346
1	J	0.60	0/1707	0.75	0/2311
1	K	0.62	0/1730	0.80	0/2342
1	L	0.58	0/1692	0.78	0/2291
All	All	0.65	0/20764	0.80	3/28115 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	LEU	CA-CB-CG	5.19	134.47	116.30
1	E	2	ASP	N-CA-C	5.16	117.57	111.33
1	F	62	VAL	N-CA-C	5.16	115.33	108.11

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	1683	0	1672	30	0
1	B	1711	0	1692	17	0
1	C	1681	0	1665	38	0
1	D	1722	0	1702	14	0
1	E	1714	0	1691	18	0
1	F	1680	0	1669	21	0
1	G	1716	0	1701	19	0
1	H	1693	0	1671	20	0
1	I	1696	0	1671	18	0
1	J	1669	0	1655	14	0
1	K	1693	0	1671	15	0
1	L	1656	0	1645	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	H	10	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	B	4	0	0	2	0
4	C	4	0	0	3	0
4	D	4	0	0	0	0
4	E	4	0	0	1	0
4	F	4	0	0	0	0
4	G	4	0	0	1	0
4	H	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	1	0
4	L	4	0	0	0	0
5	A	49	0	0	1	0
5	B	59	0	0	0	0
5	C	43	0	0	3	0
5	D	53	0	0	0	0
5	E	65	0	0	0	0
5	F	56	0	0	0	0
5	G	54	0	0	0	0
5	H	50	0	0	0	0
5	I	46	0	0	1	0
5	J	43	0	0	1	0
5	K	44	0	0	0	0
5	L	42	0	0	0	0
All	All	21039	0	20105	204	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 5.

All (204) 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:133:LEU:HD21	1:I:215:LEU:HD21	1.34	1.09
1:C:203:ILE:HD12	1:F:214:ILE:HD11	1.37	1.04
1:C:214:ILE:HD11	1:F:203:ILE:HD12	1.35	1.03
1:H:78:LEU:HD12	1:H:163:ILE:HD12	1.43	1.00
1:B:53:THR:HG22	1:D:7:LEU:HD21	1.46	0.97
1:I:133:LEU:HD23	1:I:215:LEU:HD11	1.54	0.89
1:C:214:ILE:CD1	1:F:203:ILE:HD12	2.07	0.84
1:A:183:VAL:HG12	3:A:231:SO4:O3	1.78	0.82
1:I:78:LEU:CD1	1:I:163:ILE:HD12	2.09	0.82
1:K:208:ALA:O	1:K:212:LEU:HD23	1.80	0.82
1:H:208:ALA:O	1:H:212:LEU:HD23	1.80	0.81
1:I:208:ALA:O	1:I:212:LEU:HD23	1.82	0.80
1:C:1:MET:C	5:C:273:HOH:O	2.27	0.77
1:C:198:ARG:NH2	1:C:202:GLU:OE2	2.18	0.76
1:C:1:MET:O	5:C:273:HOH:O	2.03	0.75
1:A:216:ASP:O	1:A:218:GLU:N	2.20	0.74
1:G:127:TRP:HD1	1:G:134:LEU:HD13	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:HIS:HE1	1:H:1:MET:HE1	1.53	0.74
1:I:78:LEU:HD13	1:I:163:ILE:HD12	1.67	0.74
1:D:133:LEU:C	1:D:133:LEU:HD23	2.13	0.73
1:A:7:LEU:HD21	1:C:53:THR:HG22	1.69	0.73
1:H:78:LEU:HD12	1:H:163:ILE:CD1	2.17	0.73
1:H:78:LEU:CD1	1:H:163:ILE:HD12	2.17	0.72
1:I:133:LEU:CD2	1:I:215:LEU:HD21	2.17	0.72
1:C:198:ARG:HE	1:C:201:LEU:HD23	1.55	0.71
1:J:177:HIS:HE1	1:L:1:MET:HE1	1.58	0.68
1:C:78:LEU:CD1	1:C:163:ILE:HD12	2.22	0.68
1:A:52:LEU:HD21	1:A:188:LEU:HD21	1.76	0.68
1:C:203:ILE:HD12	1:F:214:ILE:CD1	2.21	0.68
1:C:16:GLN:CA	1:C:16:GLN:HE21	2.07	0.67
1:H:127:TRP:CD1	1:H:134:LEU:HD13	2.29	0.67
1:G:137:LEU:HD11	1:G:215:LEU:HD22	1.75	0.67
1:D:116:ILE:HG13	1:D:120:LEU:HD22	1.77	0.67
1:C:16:GLN:HE21	1:C:16:GLN:HA	1.61	0.66
1:K:133:LEU:C	1:K:133:LEU:HD23	2.20	0.66
1:G:137:LEU:CD1	1:G:215:LEU:HD22	2.26	0.65
1:A:1:MET:N	5:A:271:HOH:O	2.17	0.65
1:H:133:LEU:C	1:H:133:LEU:HD23	2.21	0.64
1:G:215:LEU:HB2	1:G:220:ILE:HD11	1.80	0.64
1:C:78:LEU:HD12	1:C:163:ILE:HD12	1.80	0.63
1:A:78:LEU:HD12	1:A:163:ILE:HD12	1.81	0.62
1:K:134:LEU:HA	1:K:137:LEU:HD23	1.82	0.62
1:D:208:ALA:O	1:D:212:LEU:HD23	1.99	0.62
1:B:124:ARG:NE	3:B:232:SO4:O4	2.33	0.61
1:C:214:ILE:CG1	1:F:203:ILE:HD12	2.30	0.61
1:B:208:ALA:O	1:B:212:LEU:HD23	2.01	0.60
1:B:137:LEU:HD21	1:B:145:MET:HE2	1.83	0.60
1:H:133:LEU:HD23	1:H:133:LEU:O	2.02	0.59
1:I:69:GLN:HG2	5:I:277:HOH:O	2.01	0.59
1:E:1:MET:HE3	1:E:3:LYS:H	1.68	0.59
1:C:78:LEU:HD12	1:C:163:ILE:CD1	2.33	0.59
1:A:208:ALA:O	1:A:212:LEU:HD23	2.03	0.59
1:G:127:TRP:CD1	1:G:134:LEU:HD13	2.36	0.59
1:B:218:GLU:O	1:B:218:GLU:HG2	2.03	0.58
1:J:133:LEU:C	1:J:133:LEU:HD23	2.29	0.58
1:A:36:HIS:CD2	1:C:3:LYS:NZ	2.72	0.57
1:C:214:ILE:HD11	1:F:203:ILE:CD1	2.23	0.57
1:L:127:TRP:CD1	1:L:134:LEU:HD13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:THR:HG22	1:K:7:LEU:HD21	1.86	0.57
1:J:123:ILE:CD1	1:J:150:ASN:OD1	2.53	0.57
1:L:104:ILE:HG23	1:L:146:LEU:HD23	1.87	0.57
1:H:7:LEU:C	1:H:7:LEU:HD23	2.29	0.57
1:J:93:ILE:HG21	1:J:158:LEU:HD21	1.87	0.57
1:J:130:HIS:HA	1:J:132[B]:HIS:CE1	2.40	0.56
1:I:1:MET:HE3	1:K:92:HIS:NE2	2.21	0.56
1:I:78:LEU:CD1	1:I:163:ILE:CD1	2.83	0.55
1:L:133:LEU:C	1:L:133:LEU:HD23	2.31	0.55
1:G:208:ALA:O	1:G:212:LEU:HD23	2.07	0.55
1:B:217:GLU:HG2	1:B:218:GLU:N	2.21	0.55
1:E:15:ALA:HB3	1:G:187:PHE:CE2	2.42	0.55
1:A:36:HIS:CD2	1:C:3:LYS:HZ3	2.26	0.54
1:C:56:GLU:OE2	1:C:56:GLU:N	2.32	0.54
1:K:93:ILE:HG21	1:K:158:LEU:HD21	1.89	0.54
1:H:133:LEU:C	1:H:133:LEU:CD2	2.81	0.54
1:C:16:GLN:HA	1:C:16:GLN:NE2	2.23	0.54
1:G:7:LEU:C	1:G:7:LEU:HD23	2.33	0.54
1:I:78:LEU:HD12	1:I:163:ILE:HD12	1.88	0.54
1:E:133:LEU:C	1:E:133:LEU:HD23	2.34	0.53
1:F:177:HIS:CE1	1:H:1:MET:HE1	2.37	0.53
1:A:86:ASP:O	1:A:89:LYS:NZ	2.31	0.53
1:K:16:GLN:HE21	1:K:16:GLN:HA	1.74	0.52
1:E:53:THR:HG22	1:G:7:LEU:HD21	1.91	0.52
1:F:93:ILE:HG21	1:F:158:LEU:HD21	1.92	0.52
1:A:144:ASP:OD2	1:A:144:ASP:N	2.42	0.52
1:H:127:TRP:CD1	1:H:146:LEU:HD22	2.44	0.52
1:B:93:ILE:HG21	1:B:158:LEU:HD21	1.91	0.52
1:A:127:TRP:CD1	1:A:134:LEU:HD13	2.45	0.52
1:L:150:ASN:O	1:L:154:GLN:HG2	2.09	0.52
1:A:16:GLN:NE2	1:A:16:GLN:HA	2.25	0.51
1:B:15:ALA:HB3	1:D:187:PHE:CE2	2.45	0.51
1:C:203:ILE:CD1	1:F:214:ILE:HD11	2.26	0.51
1:B:78:LEU:HD13	1:B:163:ILE:HD12	1.93	0.51
1:D:166:SER:O	1:D:170:ARG:HG2	2.11	0.51
1:G:133:LEU:C	1:G:133:LEU:HD23	2.36	0.51
1:E:7:LEU:HD21	1:G:53:THR:HG22	1.94	0.50
1:I:150:ASN:O	1:I:154:GLN:HG2	2.11	0.50
1:I:78:LEU:HD12	1:I:163:ILE:CD1	2.40	0.50
1:C:7:LEU:HD23	1:C:7:LEU:C	2.36	0.50
1:F:202:GLU:O	1:F:206:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ALA:O	1:E:64:ARG:HA	2.12	0.50
1:B:187:PHE:CE2	1:D:15:ALA:HB3	2.47	0.49
1:C:78:LEU:CD1	1:C:163:ILE:CD1	2.89	0.49
1:A:198:ARG:NH1	1:A:201:LEU:HD23	2.28	0.49
1:D:78:LEU:HD13	1:D:163:ILE:CD1	2.43	0.49
1:F:123:ILE:CD1	1:F:150:ASN:OD1	2.61	0.49
1:C:1:MET:HA	5:C:255:HOH:O	2.12	0.49
1:K:156:TYR:HA	1:K:201:LEU:HD11	1.94	0.49
1:D:133:LEU:C	1:D:133:LEU:CD2	2.81	0.49
1:F:7:LEU:C	1:F:7:LEU:HD23	2.37	0.49
1:K:41:ALA:C	1:K:68:ASN:HB3	2.38	0.49
1:A:3:LYS:NZ	1:C:36:HIS:CD2	2.81	0.49
1:A:64:ARG:NH1	4:C:232:BCT:O3	2.46	0.48
1:G:150:ASN:O	1:G:154:GLN:HG2	2.13	0.48
1:E:1:MET:CE	1:E:3:LYS:H	2.27	0.47
1:E:93:ILE:HG21	1:E:158:LEU:HD21	1.96	0.47
1:A:133:LEU:HD21	1:A:215:LEU:HD21	1.95	0.47
1:A:78:LEU:CD1	1:A:163:ILE:HD12	2.43	0.47
1:H:150:ASN:O	1:H:154:GLN:HG2	2.14	0.47
1:I:1:MET:HE3	1:K:92:HIS:CE1	2.50	0.47
1:A:7:LEU:HD21	1:C:53:THR:CG2	2.43	0.47
1:J:7:LEU:HD21	1:L:53:THR:HG22	1.96	0.47
1:F:7:LEU:HD21	1:H:53:THR:HG22	1.96	0.46
1:B:7:LEU:HD21	1:D:53:THR:HG22	1.97	0.46
1:E:134:LEU:HA	1:E:137:LEU:HD13	1.97	0.46
1:J:112:ASP:CG	5:J:237:HOH:O	2.59	0.46
1:G:207:ASN:O	1:G:211:ARG:HG3	2.16	0.46
1:K:52:LEU:HD11	1:K:181:TYR:CE2	2.50	0.46
1:L:193:VAL:HG22	1:L:205:TYR:HA	1.98	0.46
1:K:41:ALA:HB1	4:K:232:BCT:O1	2.16	0.46
1:K:133:LEU:C	1:K:133:LEU:CD2	2.89	0.46
1:B:64:ARG:HH12	4:B:233:BCT:C	2.29	0.45
1:I:93:ILE:HG21	1:I:158:LEU:HD21	1.97	0.45
1:E:133:LEU:HD23	1:E:137:LEU:HD11	1.97	0.45
1:L:198:ARG:NH1	1:L:202:GLU:HG2	2.32	0.45
1:C:133:LEU:C	1:C:133:LEU:HD23	2.41	0.45
1:A:50:GLU:OE2	1:C:64:ARG:NH2	2.41	0.45
1:D:1:MET:HE1	1:D:3:LYS:HG3	1.97	0.45
1:B:216:ASP:O	1:B:218:GLU:N	2.50	0.45
1:D:78:LEU:HD13	1:D:163:ILE:HD12	1.97	0.44
1:G:93:ILE:HG21	1:G:158:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:133:LEU:HD23	1:J:133:LEU:O	2.16	0.44
1:C:219:ASN:CG	1:C:220:ILE:HG23	2.42	0.44
1:E:130:HIS:CD2	1:E:149:ILE:HG21	2.52	0.44
1:A:10:ASN:HB3	1:C:54:ASN:HB3	1.98	0.44
1:L:78:LEU:HD12	1:L:163:ILE:HD12	1.98	0.44
1:G:198:ARG:HE	1:G:201:LEU:HD23	1.82	0.44
1:A:150:ASN:O	1:A:154:GLN:HG2	2.17	0.44
1:B:127:TRP:CD1	1:B:134:LEU:HD13	2.53	0.44
1:J:133:LEU:HD21	1:J:145:MET:HG2	2.00	0.44
1:A:64:ARG:NH1	4:C:232:BCT:C	2.81	0.44
1:C:128:PHE:C	1:C:128:PHE:CD1	2.96	0.44
1:C:219:ASN:OD1	1:C:220:ILE:HG23	2.18	0.43
1:E:150:ASN:O	1:E:154:GLN:HG2	2.18	0.43
1:L:41:ALA:C	1:L:68:ASN:HB3	2.44	0.43
1:A:7:LEU:CD2	1:C:53:THR:HG22	2.44	0.43
1:E:71:ILE:HD12	1:E:119:TRP:CH2	2.54	0.43
1:L:78:LEU:CD1	1:L:163:ILE:HD12	2.49	0.43
1:F:156:TYR:OH	1:F:202:GLU:OE2	2.21	0.43
1:G:41:ALA:C	1:G:68:ASN:HB3	2.43	0.42
1:C:216:ASP:O	1:C:218:GLU:N	2.45	0.42
1:A:3:LYS:HZ3	1:C:36:HIS:CD2	2.37	0.42
1:E:133:LEU:C	1:E:133:LEU:CD2	2.92	0.42
1:J:7:LEU:C	1:J:7:LEU:HD23	2.44	0.42
1:C:63:HIS:HB2	1:C:80:VAL:HG11	2.01	0.42
1:E:133:LEU:HD23	1:E:137:LEU:CD1	2.50	0.42
1:J:133:LEU:C	1:J:133:LEU:CD2	2.92	0.42
1:A:64:ARG:HH11	4:C:232:BCT:C	2.32	0.42
1:F:175:SER:HA	1:F:195:ALA:O	2.19	0.42
1:E:133:LEU:CD2	1:E:137:LEU:HD11	2.49	0.42
1:H:116:ILE:HG13	1:H:120:LEU:HD22	2.01	0.42
1:A:95:ILE:HD13	1:A:154:GLN:HB3	2.01	0.42
1:A:133:LEU:HD13	1:A:149:ILE:HD11	2.01	0.42
1:B:41:ALA:HB1	4:B:233:BCT:O1	2.20	0.42
1:I:78:LEU:HD13	1:I:163:ILE:CD1	2.42	0.42
1:B:6:GLN:NE2	1:B:10:ASN:OD1	2.43	0.41
1:D:86:ASP:OD1	1:D:170:ARG:NH2	2.54	0.41
1:G:37:TYR:HB2	1:G:60:LEU:HD23	2.02	0.41
1:I:41:ALA:C	1:I:68:ASN:HB3	2.45	0.41
1:A:58:GLY:CA	1:C:46:ARG:HD3	2.50	0.41
1:C:150:ASN:O	1:C:154:GLN:HG2	2.20	0.41
1:B:18:MET:HE3	1:B:18:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASN:O	1:D:154:GLN:HG2	2.20	0.41
1:G:47:VAL:O	4:G:231:BCT:O3	2.38	0.41
1:L:116:ILE:HG13	1:L:120:LEU:HD22	2.02	0.41
1:F:16:GLN:HE21	1:F:16:GLN:HA	1.86	0.41
1:F:41:ALA:O	1:F:64:ARG:HA	2.21	0.41
1:F:3:LYS:HZ2	1:H:36:HIS:CG	2.38	0.41
1:F:98:HIS:CE1	1:F:101:CYS:HA	2.56	0.41
1:H:156:TYR:OH	1:H:202:GLU:OE2	2.21	0.41
1:J:108:MET:HA	1:J:127:TRP:CZ3	2.55	0.41
1:E:78:LEU:CD1	1:E:163:ILE:HD12	2.50	0.41
1:F:1:MET:HE1	1:F:3:LYS:HG3	2.03	0.41
1:I:140:GLU:OE1	1:I:140:GLU:N	2.38	0.41
1:K:7:LEU:C	1:K:7:LEU:HD23	2.46	0.41
1:L:133:LEU:C	1:L:133:LEU:CD2	2.93	0.41
1:E:47:VAL:O	4:E:233:BCT:O3	2.39	0.41
1:J:93:ILE:CG2	1:J:158:LEU:HD21	2.50	0.40
1:G:17:ARG:O	1:G:21:GLU:HB2	2.21	0.40
1:H:52:LEU:HD11	1:H:181:TYR:CE2	2.57	0.40
1:H:151:VAL:O	1:H:155:VAL:HG23	2.22	0.40
1:A:7:LEU:HD23	1:A:7:LEU:C	2.46	0.40
1:K:150:ASN:O	1:K:154:GLN:HG2	2.22	0.40
1:H:112:ASP:HA	1:H:117:ASN:ND2	2.36	0.40

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	206/229 (90%)	200 (97%)	5 (2%)	1 (0%)	24	21
1	B	209/229 (91%)	203 (97%)	5 (2%)	1 (0%)	24	21
1	C	205/229 (90%)	200 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	210/229 (92%)	205 (98%)	5 (2%)	0	100	100
1	E	209/229 (91%)	204 (98%)	5 (2%)	0	100	100
1	F	205/229 (90%)	201 (98%)	4 (2%)	0	100	100
1	G	210/229 (92%)	204 (97%)	6 (3%)	0	100	100
1	H	206/229 (90%)	201 (98%)	5 (2%)	0	100	100
1	I	207/229 (90%)	199 (96%)	7 (3%)	1 (0%)	24	21
1	J	203/229 (89%)	196 (97%)	7 (3%)	0	100	100
1	K	206/229 (90%)	202 (98%)	4 (2%)	0	100	100
1	L	202/229 (88%)	199 (98%)	3 (2%)	0	100	100
All	All	2478/2748 (90%)	2414 (97%)	61 (2%)	3 (0%)	48	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	GLU
1	B	217	GLU
1	I	219	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	183/201 (91%)	176 (96%)	7 (4%)	29	29
1	B	185/201 (92%)	179 (97%)	6 (3%)	34	35
1	C	182/201 (90%)	175 (96%)	7 (4%)	29	29
1	D	186/201 (92%)	177 (95%)	9 (5%)	23	21
1	E	185/201 (92%)	176 (95%)	9 (5%)	22	20
1	F	181/201 (90%)	173 (96%)	8 (4%)	25	24
1	G	185/201 (92%)	178 (96%)	7 (4%)	29	29
1	H	183/201 (91%)	178 (97%)	5 (3%)	39	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	182/201 (90%)	177 (97%)	5 (3%)	39	42
1	J	180/201 (90%)	172 (96%)	8 (4%)	25	24
1	K	183/201 (91%)	175 (96%)	8 (4%)	25	24
1	L	179/201 (89%)	175 (98%)	4 (2%)	45	50
All	All	2194/2412 (91%)	2111 (96%)	83 (4%)	29	29

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	18	MET
1	A	46	ARG
1	A	52	LEU
1	A	133	LEU
1	A	144	ASP
1	A	183	VAL
1	B	18	MET
1	B	78	LEU
1	B	100	ASN
1	B	110	ASP
1	B	133	LEU
1	B	218	GLU
1	C	16	GLN
1	C	56	GLU
1	C	133	LEU
1	C	211	ARG
1	C	212	LEU
1	C	217	GLU
1	C	219	ASN
1	D	18	MET
1	D	21	GLU
1	D	33	GLN
1	D	78	LEU
1	D	110	ASP
1	D	120	LEU
1	D	133	LEU
1	D	217	GLU
1	D	218	GLU
1	E	1	MET
1	E	18	MET
1	E	78	LEU

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Mol	Chain	Res	Type
1	E	110	ASP
1	E	133	LEU
1	E	202	GLU
1	E	211	ARG
1	E	212	LEU
1	E	218	GLU
1	F	18	MET
1	F	33	GLN
1	F	51	LYS
1	F	73	THR
1	F	78	LEU
1	F	133	LEU
1	F	137	LEU
1	F	211	ARG
1	G	18	MET
1	G	33	GLN
1	G	78	LEU
1	G	137	LEU
1	G	198	ARG
1	G	218	GLU
1	G	221	LEU
1	H	18	MET
1	H	21	GLU
1	H	120	LEU
1	H	133	LEU
1	H	202	GLU
1	I	18	MET
1	I	33	GLN
1	I	54	ASN
1	I	133	LEU
1	I	202	GLU
1	J	1	MET
1	J	18	MET
1	J	78	LEU
1	J	133	LEU
1	J	137	LEU
1	J	198	ARG
1	J	211	ARG
1	J	212	LEU
1	K	1	MET
1	K	16	GLN
1	K	18	MET

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Mol	Chain	Res	Type
1	K	110	ASP
1	K	123	ILE
1	K	133	LEU
1	K	202	GLU
1	K	218	GLU
1	L	120	LEU
1	L	169	GLU
1	L	212	LEU
1	L	216	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	16	GLN
1	A	117	ASN
1	B	16	GLN
1	B	33	GLN
1	B	100	ASN
1	B	191	GLN
1	C	16	GLN
1	C	100	ASN
1	D	33	GLN
1	D	54	ASN
1	D	117	ASN
1	D	191	GLN
1	D	219	ASN
1	E	16	GLN
1	E	54	ASN
1	E	184	ASN
1	E	219	ASN
1	F	6	GLN
1	F	16	GLN
1	F	54	ASN
1	G	54	ASN
1	G	191	GLN
1	H	16	GLN
1	H	54	ASN
1	I	16	GLN
1	I	33	GLN
1	I	54	ASN
1	I	132	HIS

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Mol	Chain	Res	Type
1	J	6	GLN
1	J	16	GLN
1	J	54	ASN
1	K	16	GLN
1	K	54	ASN
1	K	191	GLN
1	L	33	GLN
1	L	54	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 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	$\# Z > 2$
3	SO4	A	231	-	4,4,4	0.28	0	6,6,6	0.23	0
4	BCT	G	231	-	3,3,3	0.48	0	2,3,3	0.33	0
3	SO4	E	232	-	4,4,4	0.27	0	6,6,6	0.46	0
3	SO4	D	231	-	4,4,4	0.25	0	6,6,6	0.46	0
3	SO4	B	232	-	4,4,4	0.29	0	6,6,6	0.33	0
3	SO4	I	231	-	4,4,4	0.20	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BCT	K	232	-	3,3,3	0.54	0	2,3,3	0.22	0
3	SO4	E	231	-	4,4,4	0.24	0	6,6,6	0.48	0
4	BCT	D	232	-	3,3,3	0.53	0	2,3,3	0.47	0
4	BCT	I	232	-	3,3,3	0.59	0	2,3,3	0.45	0
3	SO4	B	231	-	4,4,4	0.26	0	6,6,6	0.35	0
3	SO4	L	231	-	4,4,4	0.27	0	6,6,6	0.38	0
4	BCT	F	231	-	3,3,3	0.45	0	2,3,3	0.88	0
4	BCT	H	233	-	3,3,3	0.42	0	2,3,3	0.44	0
3	SO4	J	231	-	4,4,4	0.27	0	6,6,6	0.46	0
4	BCT	C	232	-	3,3,3	0.68	0	2,3,3	0.59	0
4	BCT	B	233	-	3,3,3	0.50	0	2,3,3	0.31	0
3	SO4	C	231	-	4,4,4	0.26	0	6,6,6	0.24	0
3	SO4	H	231	-	4,4,4	0.28	0	6,6,6	0.44	0
4	BCT	E	233	-	3,3,3	0.54	0	2,3,3	0.77	0
3	SO4	K	231	-	4,4,4	0.28	0	6,6,6	0.32	0
4	BCT	J	232	-	3,3,3	0.55	0	2,3,3	0.34	0
4	BCT	L	232	-	3,3,3	0.49	0	2,3,3	0.11	0
3	SO4	H	232	-	4,4,4	0.27	0	6,6,6	0.37	0

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.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	231	SO4	1	0
4	G	231	BCT	1	0
3	B	232	SO4	1	0
4	K	232	BCT	1	0
4	C	232	BCT	3	0
4	B	233	BCT	2	0
4	E	233	BCT	1	0

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	208/229 (90%)	0.87	24 (11%) 9 8	21, 34, 48, 57	2 (0%)
1	B	212/229 (92%)	0.71	24 (11%) 10 9	21, 33, 46, 51	1 (0%)
1	C	208/229 (90%)	0.86	26 (12%) 8 7	20, 33, 48, 54	1 (0%)
1	D	213/229 (93%)	1.02	33 (15%) 5 4	20, 33, 45, 52	1 (0%)
1	E	212/229 (92%)	1.21	37 (17%) 4 3	19, 32, 44, 48	1 (0%)
1	F	208/229 (90%)	0.89	27 (12%) 7 6	16, 32, 44, 51	1 (0%)
1	G	214/229 (93%)	1.44	50 (23%) 2 2	27, 34, 46, 49	0
1	H	209/229 (91%)	1.04	26 (12%) 8 7	21, 34, 46, 60	1 (0%)
1	I	210/229 (91%)	2.11	112 (53%) 0 0	22, 37, 50, 54	1 (0%)
1	J	205/229 (89%)	1.04	33 (16%) 4 4	18, 35, 47, 53	2 (0%)
1	K	209/229 (91%)	2.63	148 (70%) 0 0	22, 38, 49, 55	1 (0%)
1	L	206/229 (89%)	1.05	20 (9%) 13 12	30, 36, 47, 50	0
All	All	2514/2748 (91%)	1.24	560 (22%) 2 2	16, 34, 47, 60	12 (0%)

All (560) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	128[A]	PHE	12.9
1	J	128[A]	PHE	8.3
1	E	128[A]	PHE	7.8
1	H	128[A]	PHE	7.6
1	I	128[A]	PHE	7.6
1	F	128[A]	PHE	6.6
1	D	128[A]	PHE	6.5
1	I	219	ASN	6.1
1	J	132[A]	HIS	6.1
1	I	220	ILE	6.0
1	A	219	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	219	ASN	5.6
1	K	187	PHE	5.4
1	K	135	GLY	5.2
1	K	133	LEU	5.2
1	B	128[A]	PHE	5.1
1	A	220	ILE	5.0
1	K	112	ASP	5.0
1	I	20	GLU	5.0
1	C	220	ILE	5.0
1	I	187	PHE	5.0
1	E	20	GLU	4.9
1	L	128	PHE	4.9
1	K	139	PRO	4.7
1	I	7	LEU	4.7
1	C	132[A]	HIS	4.7
1	H	219	ASN	4.7
1	I	215	LEU	4.7
1	K	53	THR	4.6
1	K	1	MET	4.6
1	K	116	ILE	4.6
1	K	109	ALA	4.6
1	F	31	ASP	4.6
1	G	128	PHE	4.6
1	H	216	ASP	4.5
1	F	112	ASP	4.5
1	A	217	GLU	4.5
1	H	217	GLU	4.5
1	F	33	GLN	4.4
1	D	220	ILE	4.4
1	K	168	TRP	4.4
1	K	33	GLN	4.4
1	K	21	GLU	4.4
1	K	56	GLU	4.4
1	E	12	TYR	4.3
1	I	56	GLU	4.3
1	I	12	TYR	4.2
1	K	205	TYR	4.2
1	C	57	PRO	4.2
1	I	84	ALA	4.2
1	K	134	LEU	4.2
1	K	123	ILE	4.1
1	K	212	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	107	ALA	4.1
1	K	32	HIS	4.1
1	K	119	TRP	4.0
1	G	7	LEU	4.0
1	K	115	LEU	4.0
1	I	19	LYS	4.0
1	G	221	LEU	3.9
1	G	219	ASN	3.9
1	G	12	TYR	3.9
1	K	17	ARG	3.9
1	K	78	LEU	3.9
1	K	113	LEU	3.9
1	K	182	ASP	3.8
1	K	126	ILE	3.8
1	K	54	ASN	3.8
1	K	184	ASN	3.8
1	F	140	GLU	3.8
1	K	51	LYS	3.8
1	L	138	SER	3.8
1	K	73	THR	3.8
1	D	135	GLY	3.8
1	K	206	ARG	3.8
1	K	71	ILE	3.7
1	K	138	SER	3.7
1	C	181	TYR	3.7
1	L	127	TRP	3.7
1	K	137	LEU	3.7
1	K	100	ASN	3.7
1	B	217	GLU	3.7
1	E	187	PHE	3.6
1	I	75	PHE	3.6
1	I	9	ALA	3.6
1	A	56	GLU	3.6
1	K	59	GLU	3.6
1	G	189	VAL	3.6
1	K	156	TYR	3.6
1	E	211	ARG	3.6
1	K	136	LYS	3.6
1	K	127	TRP	3.6
1	K	214	ILE	3.6
1	G	206	ARG	3.6
1	I	119	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	16	GLN	3.5
1	A	144	ASP	3.5
1	G	31	ASP	3.5
1	H	110	ASP	3.5
1	L	216	ASP	3.5
1	K	199	GLU	3.5
1	I	34	THR	3.5
1	C	1	MET	3.5
1	D	218	GLU	3.5
1	I	8	PHE	3.5
1	B	219	ASN	3.5
1	I	11	ASN	3.5
1	K	8	PHE	3.4
1	K	2	ASP	3.4
1	H	206	ARG	3.4
1	H	127	TRP	3.4
1	I	15	ALA	3.4
1	H	218	GLU	3.4
1	I	73	THR	3.4
1	K	147	THR	3.4
1	D	110	ASP	3.4
1	H	199	GLU	3.4
1	K	67	ALA	3.4
1	K	210	ALA	3.4
1	I	164	VAL	3.4
1	I	183	VAL	3.4
1	I	16	GLN	3.4
1	K	120	LEU	3.4
1	C	56	GLU	3.3
1	J	16	GLN	3.3
1	G	199	GLU	3.3
1	K	18	MET	3.3
1	J	112	ASP	3.3
1	E	37	TYR	3.3
1	K	90	ILE	3.3
1	J	137	LEU	3.3
1	I	218	GLU	3.3
1	K	39	TRP	3.3
1	L	33	GLN	3.3
1	G	183	VAL	3.3
1	K	151	VAL	3.3
1	L	20	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	14	TRP	3.2
1	K	20	GLU	3.2
1	E	1	MET	3.2
1	J	1	MET	3.2
1	K	16	GLN	3.2
1	K	75	PHE	3.2
1	K	211	ARG	3.2
1	F	12	TYR	3.2
1	H	215	LEU	3.2
1	K	12	TYR	3.2
1	E	110	ASP	3.2
1	G	56	GLU	3.2
1	K	208	ALA	3.1
1	K	7	LEU	3.1
1	K	55	LEU	3.1
1	J	20	GLU	3.1
1	E	8	PHE	3.1
1	F	1	MET	3.1
1	G	1	MET	3.1
1	C	198	ARG	3.1
1	I	81	VAL	3.1
1	B	169	GLU	3.1
1	K	132	HIS	3.1
1	K	219	ASN	3.1
1	I	17	ARG	3.1
1	I	112	ASP	3.1
1	I	163	ILE	3.1
1	J	33	GLN	3.1
1	K	6	GLN	3.1
1	B	1	MET	3.1
1	G	168	TRP	3.0
1	K	76	ASN	3.0
1	I	74	ASP	3.0
1	I	144	ASP	3.0
1	G	15	ALA	3.0
1	C	45	SER	3.0
1	I	3	LYS	3.0
1	K	118	ASN	3.0
1	D	199	GLU	3.0
1	A	182	ASP	3.0
1	I	5	LYS	3.0
1	I	14	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	168	TRP	3.0
1	I	216	ASP	3.0
1	K	111	LYS	3.0
1	K	129	LYS	3.0
1	K	165	LYS	3.0
1	G	85	VAL	3.0
1	I	121	LEU	3.0
1	K	70	VAL	3.0
1	K	130	HIS	3.0
1	J	107	ALA	2.9
1	E	115	LEU	2.9
1	I	212	LEU	2.9
1	K	121	LEU	2.9
1	D	132	HIS	2.9
1	I	33	GLN	2.9
1	K	197	SER	2.9
1	A	184	ASN	2.9
1	K	117	ASN	2.9
1	I	77	CYS	2.9
1	I	188	LEU	2.9
1	E	112	ASP	2.9
1	I	71	ILE	2.9
1	B	198	ARG	2.9
1	A	218	GLU	2.9
1	K	37	TYR	2.9
1	D	219	ASN	2.9
1	E	19	LYS	2.9
1	F	137	LEU	2.9
1	E	31	ASP	2.9
1	F	110	ASP	2.9
1	K	161	THR	2.9
1	F	199	GLU	2.9
1	L	169	GLU	2.9
1	C	110	ASP	2.8
1	J	133	LEU	2.8
1	K	38	LEU	2.8
1	K	47	VAL	2.8
1	G	139	PRO	2.8
1	E	132	HIS	2.8
1	H	33	GLN	2.8
1	H	132	HIS	2.8
1	H	169	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	4	ILE	2.8
1	D	100	ASN	2.8
1	I	6	GLN	2.8
1	K	144	ASP	2.8
1	A	181	TYR	2.8
1	B	12	TYR	2.8
1	C	218	GLU	2.8
1	K	106	ALA	2.8
1	K	155	VAL	2.8
1	I	54	ASN	2.8
1	C	46	ARG	2.8
1	H	138	SER	2.8
1	I	13	SER	2.8
1	A	216	ASP	2.8
1	D	56	GLU	2.8
1	J	12	TYR	2.8
1	B	212	LEU	2.8
1	K	87	VAL	2.8
1	G	220	ILE	2.8
1	K	124	ARG	2.7
1	K	160	ARG	2.7
1	G	132	HIS	2.7
1	K	108	MET	2.7
1	A	112	ASP	2.7
1	I	169	GLU	2.7
1	G	121	LEU	2.7
1	I	37	TYR	2.7
1	C	34	THR	2.7
1	A	57	PRO	2.7
1	I	211	ARG	2.7
1	G	33	GLN	2.7
1	J	214	ILE	2.7
1	B	110	ASP	2.7
1	E	9	ALA	2.7
1	K	167	ALA	2.7
1	F	113	LEU	2.7
1	K	181	TYR	2.7
1	D	169	GLU	2.7
1	I	166	SER	2.7
1	G	212	LEU	2.7
1	I	88	LEU	2.7
1	I	133	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	134	LEU	2.7
1	I	161	THR	2.7
1	E	218	GLU	2.7
1	I	35	PRO	2.7
1	G	156	TYR	2.7
1	I	184	ASN	2.7
1	B	33	GLN	2.6
1	B	9	ALA	2.6
1	B	199	GLU	2.6
1	I	49	ALA	2.6
1	J	106	ALA	2.6
1	K	10	ASN	2.6
1	J	2	ASP	2.6
1	I	80	VAL	2.6
1	K	66	VAL	2.6
1	L	183	VAL	2.6
1	A	206	ARG	2.6
1	I	58	GLY	2.6
1	J	56	GLU	2.6
1	D	1	MET	2.6
1	K	145	MET	2.6
1	K	122	HIS	2.6
1	I	139	PRO	2.6
1	J	212	LEU	2.6
1	I	138	SER	2.6
1	G	4	ILE	2.6
1	I	159	GLY	2.6
1	I	100	ASN	2.6
1	K	207	ASN	2.6
1	K	9	ALA	2.6
1	K	200	THR	2.6
1	K	48	PRO	2.6
1	G	112	ASP	2.6
1	G	214	ILE	2.6
1	L	135	GLY	2.6
1	I	48	PRO	2.6
1	I	110	ASP	2.6
1	L	112	ASP	2.6
1	E	52	LEU	2.6
1	K	179	TRP	2.6
1	B	16	GLN	2.5
1	G	21	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	183	VAL	2.5
1	I	116	ILE	2.5
1	K	189	VAL	2.5
1	D	12	TYR	2.5
1	F	100	ASN	2.5
1	A	198	ARG	2.5
1	J	198	ARG	2.5
1	F	109	ALA	2.5
1	I	79	SER	2.5
1	D	137	LEU	2.5
1	D	215	LEU	2.5
1	E	215	LEU	2.5
1	B	21	GLU	2.5
1	K	159	GLY	2.5
1	K	209	ILE	2.5
1	K	190	ASP	2.5
1	A	7	LEU	2.5
1	B	7	LEU	2.5
1	A	105	HIS	2.5
1	I	32	HIS	2.5
1	K	114	GLY	2.5
1	I	189	VAL	2.5
1	K	163	ILE	2.5
1	K	198	ARG	2.5
1	G	205	TYR	2.5
1	A	110	ASP	2.5
1	D	2	ASP	2.5
1	H	20	GLU	2.5
1	J	169	GLU	2.5
1	J	199	GLU	2.5
1	K	217	GLU	2.5
1	G	73	THR	2.5
1	I	106	ALA	2.5
1	C	215	LEU	2.5
1	D	212	LEU	2.5
1	I	78	LEU	2.5
1	J	113	LEU	2.5
1	A	132[A]	HIS	2.5
1	F	32	HIS	2.5
1	K	142	ARG	2.5
1	K	157	ASN	2.5
1	A	80	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	87	VAL	2.4
1	K	104	ILE	2.5
1	K	180	VAL	2.4
1	I	2	ASP	2.4
1	K	140	GLU	2.4
1	J	215	LEU	2.4
1	G	160	ARG	2.4
1	A	128	PHE	2.4
1	I	76	ASN	2.4
1	C	217	GLU	2.4
1	C	216	ASP	2.4
1	F	2	ASP	2.4
1	G	110	ASP	2.4
1	I	40	ILE	2.4
1	I	44	ASP	2.4
1	K	85	VAL	2.4
1	I	45	SER	2.4
1	I	162	SER	2.4
1	H	139	PRO	2.4
1	I	57	PRO	2.4
1	B	17	ARG	2.4
1	I	136	LYS	2.4
1	E	137	LEU	2.4
1	I	72	HIS	2.4
1	I	103	GLY	2.4
1	I	123	ILE	2.4
1	I	126	ILE	2.4
1	I	180	VAL	2.4
1	I	214	ILE	2.4
1	B	206	ARG	2.4
1	G	17	ARG	2.4
1	D	133	LEU	2.4
1	G	134	LEU	2.4
1	I	82	GLN	2.4
1	F	116	ILE	2.4
1	J	116	ILE	2.4
1	K	203	ILE	2.4
1	A	46	ARG	2.4
1	I	160	ARG	2.4
1	K	105	HIS	2.4
1	D	30	ALA	2.3
1	F	21	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	107	ALA	2.3
1	J	109	ALA	2.3
1	K	218	GLU	2.3
1	D	7	LEU	2.3
1	K	188	LEU	2.3
1	E	214	ILE	2.3
1	K	40	ILE	2.3
1	I	217	GLU	2.3
1	L	57	PRO	2.3
1	D	15	ALA	2.3
1	F	9	ALA	2.3
1	F	107	ALA	2.3
1	G	133	LEU	2.3
1	K	215	LEU	2.3
1	K	125	ASP	2.3
1	K	216	ASP	2.3
1	G	8	PHE	2.3
1	K	204	SER	2.3
1	F	132	HIS	2.3
1	I	4	ILE	2.3
1	A	183	VAL	2.3
1	F	169	GLU	2.3
1	I	21	GLU	2.3
1	B	100	ASN	2.3
1	E	30	ALA	2.3
1	I	167	ALA	2.3
1	F	29	LEU	2.3
1	G	2	ASP	2.3
1	G	127	TRP	2.3
1	I	156	TYR	2.3
1	H	211	ARG	2.3
1	K	131	GLY	2.3
1	K	158	LEU	2.3
1	D	18	MET	2.3
1	I	1	MET	2.3
1	B	56	GLU	2.3
1	D	187	PHE	2.3
1	F	56	GLU	2.3
1	K	61	PHE	2.3
1	L	56	GLU	2.3
1	D	33	GLN	2.3
1	B	57	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	53	THR	2.3
1	I	101	CYS	2.3
1	F	3	LYS	2.3
1	L	110	ASP	2.3
1	H	108	MET	2.3
1	I	115	LEU	2.3
1	K	174	LEU	2.3
1	I	83	TYR	2.3
1	K	83	TYR	2.3
1	D	20	GLU	2.2
1	I	199	GLU	2.2
1	K	92	HIS	2.2
1	K	154	GLN	2.2
1	I	61	PHE	2.2
1	E	206	ARG	2.2
1	I	142	ARG	2.2
1	I	198	ARG	2.2
1	J	117	ASN	2.2
1	L	211	ARG	2.2
1	H	136	LYS	2.2
1	C	112	ASP	2.2
1	G	109	ALA	2.2
1	C	133	LEU	2.2
1	D	29	LEU	2.2
1	E	88	LEU	2.2
1	K	52	LEU	2.2
1	J	140	GLU	2.2
1	K	153	GLU	2.2
1	C	105	HIS	2.2
1	D	6	GLN	2.2
1	A	34	THR	2.2
1	G	54	ASN	2.2
1	C	183	VAL	2.2
1	G	111	LYS	2.2
1	K	93	ILE	2.2
1	K	149	ILE	2.2
1	K	193	VAL	2.2
1	K	110	ASP	2.2
1	K	103	GLY	2.2
1	G	106	ALA	2.2
1	K	49	ALA	2.2
1	H	212	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	55	LEU	2.2
1	J	7	LEU	2.2
1	L	133	LEU	2.2
1	E	54	ASN	2.2
1	D	216	ASP	2.2
1	G	126	ILE	2.2
1	G	182	ASP	2.2
1	E	189	VAL	2.2
1	K	91	GLU	2.2
1	K	172	GLN	2.2
1	L	215	LEU	2.2
1	E	138	SER	2.2
1	G	198	ARG	2.2
1	I	181	TYR	2.2
1	J	136	LYS	2.2
1	E	100	ASN	2.2
1	L	1	MET	2.2
1	C	182	ASP	2.2
1	E	216	ASP	2.2
1	E	4	ILE	2.1
1	I	131	GLY	2.1
1	K	186	GLY	2.1
1	K	195	ALA	2.1
1	D	211	ARG	2.1
1	E	7	LEU	2.1
1	B	138	SER	2.1
1	C	100	ASN	2.1
1	E	219	ASN	2.1
1	F	108	MET	2.1
1	B	20	GLU	2.1
1	E	21	GLU	2.1
1	F	20	GLU	2.1
1	H	135	GLY	2.1
1	I	114	GLY	2.1
1	I	135	GLY	2.1
1	L	32	HIS	2.1
1	E	15	ALA	2.1
1	H	167	ALA	2.1
1	B	215	LEU	2.1
1	K	201	LEU	2.1
1	L	113	LEU	2.1
1	K	77	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	79	SER	2.1
1	E	18	MET	2.1
1	J	110	ASP	2.1
1	J	139	PRO	2.1
1	D	71	ILE	2.1
1	I	94	ILE	2.1
1	K	192	GLY	2.1
1	I	70	VAL	2.1
1	I	85	VAL	2.1
1	L	111	LYS	2.1
1	A	109	ALA	2.1
1	G	210	ALA	2.1
1	K	15	ALA	2.1
1	K	152	ALA	2.1
1	E	133	LEU	2.1
1	G	78	LEU	2.1
1	I	113	LEU	2.1
1	J	115	LEU	2.1
1	G	18	MET	2.1
1	J	101	CYS	2.1
1	C	2	ASP	2.1
1	C	16	GLN	2.1
1	K	69	GLN	2.1
1	J	105	HIS	2.1
1	D	136	LYS	2.1
1	I	209	ILE	2.1
1	C	128	PHE	2.1
1	E	75	PHE	2.1
1	G	14	TRP	2.1
1	I	50	GLU	2.0
1	K	194	MET	2.0
1	K	74	ASP	2.0
1	J	32	HIS	2.0
1	D	8	PHE	2.0
1	H	84	ALA	2.0
1	H	210	ALA	2.0
1	H	137	LEU	2.0
1	B	112	ASP	2.0
1	E	2	ASP	2.0
1	C	17	ARG	2.0
1	I	132	HIS	2.0
1	F	139	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	171	GLY	2.0
1	G	159	GLY	2.0
1	I	205	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
3	SO4	K	231	5/5	0.52	0.20	89,91,91,91	0
3	SO4	E	232	5/5	0.53	0.20	73,74,75,76	0
3	SO4	H	232	5/5	0.62	0.23	75,78,78,79	0
3	SO4	L	231	5/5	0.68	0.19	75,77,77,78	0
3	SO4	H	231	5/5	0.71	0.17	71,73,74,75	0
3	SO4	I	231	5/5	0.72	0.17	73,74,75,76	0
4	BCT	C	232	4/4	0.75	0.15	18,19,19,20	4
3	SO4	J	231	5/5	0.79	0.15	72,72,74,74	0
3	SO4	E	231	5/5	0.83	0.15	64,67,68,68	0
4	BCT	G	231	4/4	0.84	0.17	40,40,40,40	0
4	BCT	K	232	4/4	0.85	0.17	37,38,38,38	0
3	SO4	D	231	5/5	0.89	0.12	67,69,70,70	0
4	BCT	E	233	4/4	0.89	0.17	38,38,38,39	0
3	SO4	B	231	5/5	0.90	0.10	57,59,60,60	0
3	SO4	C	231	5/5	0.90	0.11	60,62,62,62	0
4	BCT	D	232	4/4	0.90	0.13	41,41,41,42	0
4	BCT	B	233	4/4	0.91	0.12	45,46,46,46	0
4	BCT	I	232	4/4	0.91	0.16	43,44,44,45	0
3	SO4	A	231	5/5	0.91	0.16	38,38,39,39	5
3	SO4	B	232	5/5	0.93	0.11	55,55,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BCT	J	232	4/4	0.94	0.14	41,41,42,42	0
4	BCT	F	231	4/4	0.94	0.12	38,38,38,38	0
4	BCT	L	232	4/4	0.94	0.16	41,41,41,41	0
2	ZN	K	230	1/1	0.95	0.15	36,36,36,36	0
2	ZN	I	230	1/1	0.95	0.12	36,36,36,36	0
2	ZN	A	230	1/1	0.96	0.10	31,31,31,31	0
2	ZN	C	230	1/1	0.96	0.09	32,32,32,32	0
2	ZN	G	230	1/1	0.96	0.15	31,31,31,31	0
4	BCT	H	233	4/4	0.96	0.13	38,38,38,39	0
2	ZN	B	230	1/1	0.97	0.09	31,31,31,31	0
2	ZN	L	230	1/1	0.97	0.10	32,32,32,32	0
2	ZN	E	230	1/1	0.98	0.14	28,28,28,28	0
2	ZN	J	230	1/1	0.98	0.07	33,33,33,33	0
2	ZN	D	230	1/1	0.98	0.08	30,30,30,30	0
2	ZN	H	230	1/1	0.98	0.08	32,32,32,32	0
2	ZN	F	230	1/1	0.99	0.08	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.