Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 12:45 PM EDT

|		
PDB ID	:	2A8C
Title	:	Haemophilus influenzae beta-carbonic anhydrase
Authors	:	Cronk, J.D.; Rowlett, R.S.; Zhang, K.Y.J.; Tu, C.; Endrizzi, J.A.; Lee, J.; Gareiss, P.C.; Preiss, J.R.
Deposited on	:	2005-07-07
Resolution	:	2.30 Å(reported)

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 2.30 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		15
Ramachandran outliers		1.0%
Sidechain outliers		3.7%
RSRZ outliers		12.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
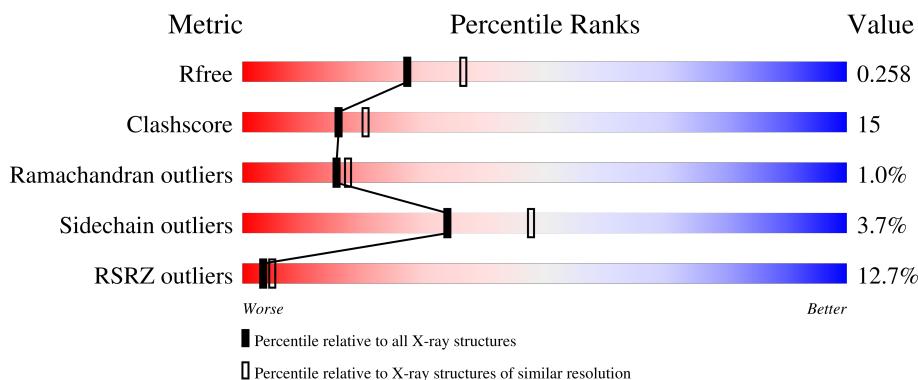
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	12% / 74% / 21% · ·
1	B	229	12% / 71% / 24% · ·
1	C	229	12% / 58% / 34% · ·
1	D	229	7% / 67% / 26% · 6%
1	E	229	17% / 57% / 35% · ·
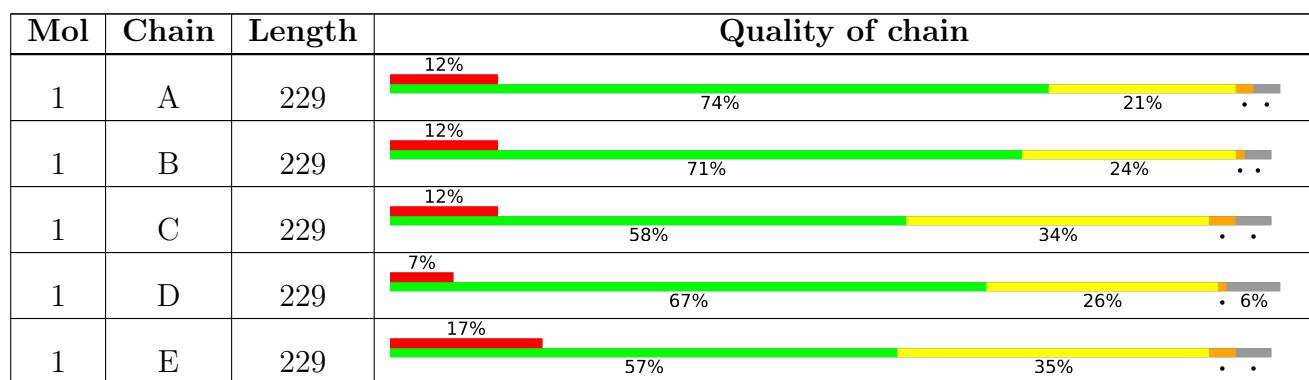
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Mol	Chain	Length	Quality of chain
1	F	229	

13%

71%   24%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10789 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	221	Total	C	N	O	S	0	0	0
			1780	1130	315	326	9			
1	B	221	Total	C	N	O	S	0	0	0
			1780	1130	315	326	9			
1	C	219	Total	C	N	O	S	0	0	0
			1764	1118	313	324	9			
1	D	215	Total	C	N	O	S	0	0	0
			1730	1100	308	313	9			
1	E	220	Total	C	N	O	S	0	0	0
			1772	1124	314	325	9			
1	F	219	Total	C	N	O	S	0	0	0
			1764	1118	313	324	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
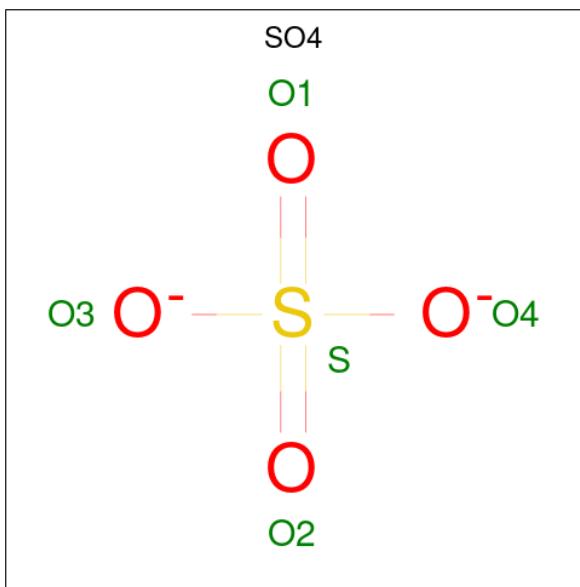
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	29	Total 29	O 29	0	0
4	C	25	Total 25	O 25	0	0
4	D	32	Total 32	O 32	0	0
4	E	16	Total 16	O 16	0	0
4	F	28	Total 28	O 28	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Carbonic anhydrase 2
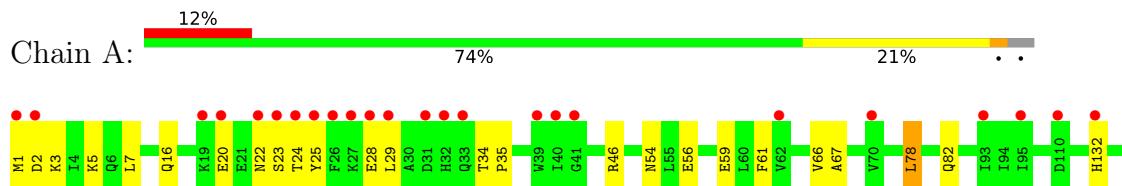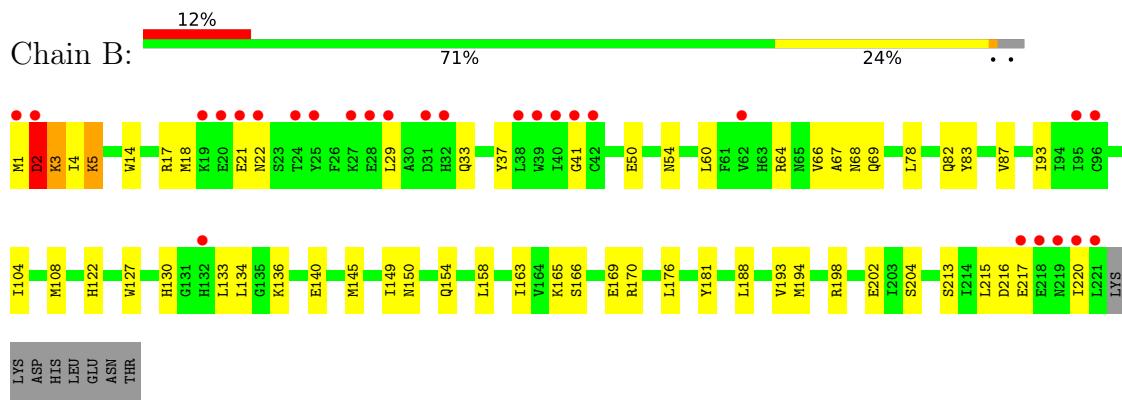
Chain A:

- Molecule 1: Carbonic anhydrase 2

Chain B:

- Molecule 1: Carbonic anhydrase 2

Chain C:

• Molecule 1: Carbonic anhydrase 2

Chain D:

• Molecule 1: Carbonic anhydrase 2

Chain E:

• Molecule 1: Carbonic anhydrase 2

Chain F:
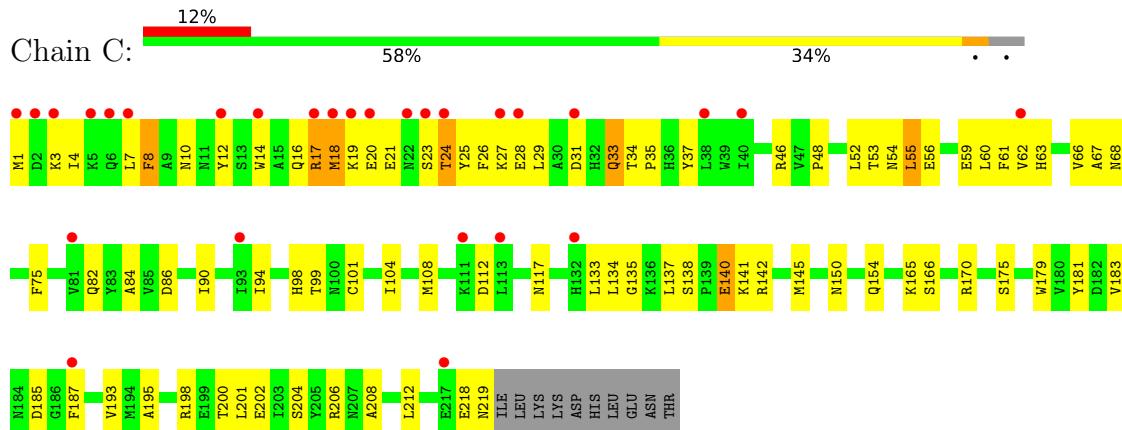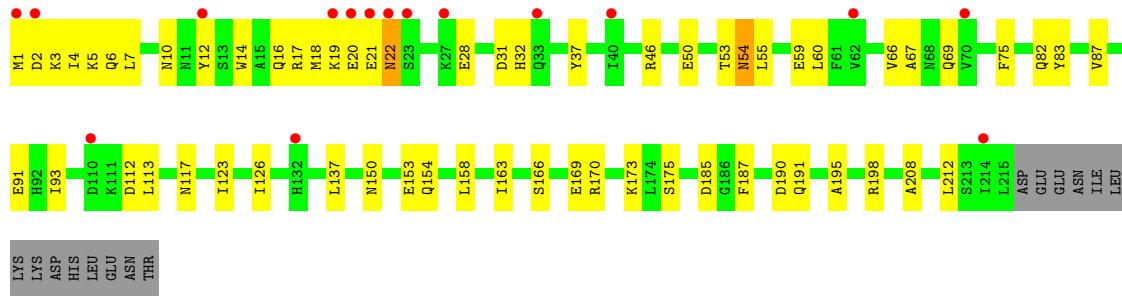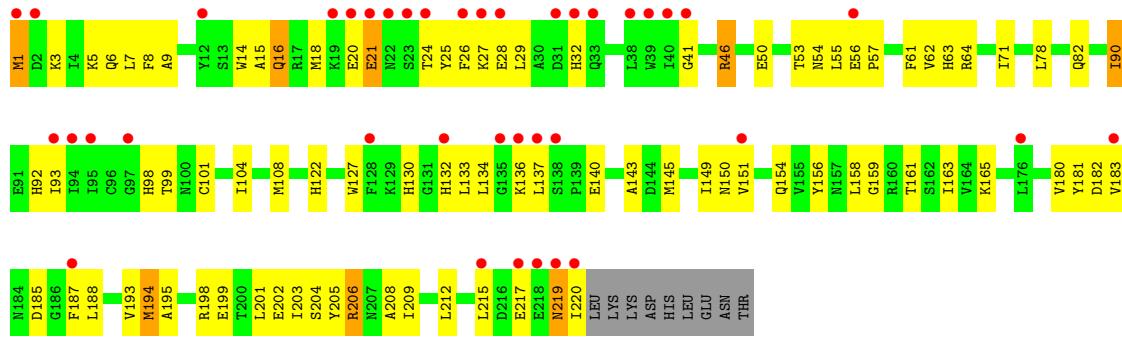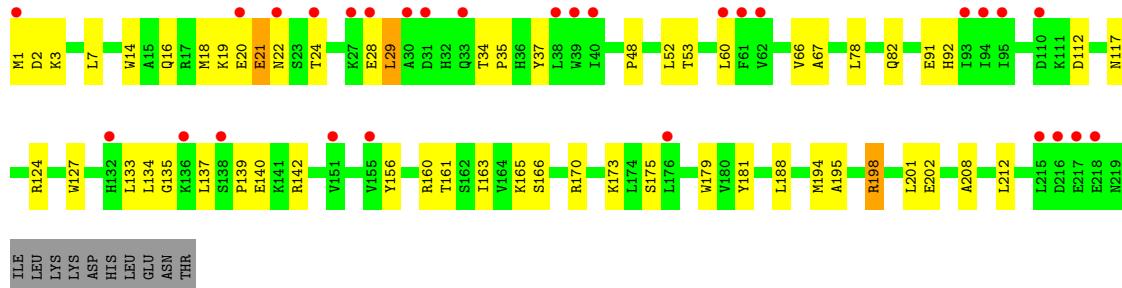
4 Data and refinement statistics ⓘ

| Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	232.66Å 144.73Å 52.41Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 24.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.7 (25.00-2.30) 85.4 (24.92-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.28Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.259 0.215 , 0.258	Depositor DCC
R_{free} test set	3329 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10789	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, SO4

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	0.37	0/1819	0.60	1/2464 (0.0%)
1	B	0.35	0/1819	0.57	0/2464
1	C	0.33	0/1803	0.57	1/2442 (0.0%)
1	D	0.36	0/1769	0.58	0/2396
1	E	0.33	0/1811	0.58	1/2453 (0.0%)
1	F	0.34	0/1803	0.57	0/2442
All	All	0.35	0/10824	0.58	3/14661 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	PHE	N-CA-C	-5.34	96.59	111.00
1	C	61	PHE	N-CA-C	-5.30	96.67	111.00
1	E	61	PHE	N-CA-C	-5.30	96.68	111.00

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	1780	0	1759	38	0
1	B	1780	0	1759	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1764	0	1737	75	0
1	D	1730	0	1715	51	0
1	E	1772	0	1748	79	0
1	F	1764	0	1737	50	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
3	B	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	1	0
4	A	33	0	0	0	0
4	B	29	0	0	0	0
4	C	25	0	0	0	0
4	D	32	0	0	2	0
4	E	16	0	0	1	0
4	F	28	0	0	2	0
All	All	10789	0	10455	307	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 15.

All (307) 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:F:1:MET:HG2	1:F:2:ASP:H	1.22	1.01
1:F:1:MET:HE2	1:F:3:LYS:H	1.39	0.87
1:F:198:ARG:NH1	1:F:202:GLU:HG2	1.95	0.81
1:E:16:GLN:HE21	1:E:16:GLN:HA	1.46	0.80
1:D:113:LEU:H	1:D:117:ASN:HD21	1.27	0.80
1:D:82:GLN:HB2	1:D:163:ILE:HD13	1.65	0.78
1:A:78:LEU:HD12	1:A:163:ILE:HD12	1.64	0.77
1:F:1:MET:HG2	1:F:2:ASP:N	1.99	0.77
1:A:1:MET:HG3	1:A:2:ASP:N	2.00	0.77
1:F:208:ALA:O	1:F:212:LEU:HD23	1.84	0.77
1:C:24:THR:HA	1:C:27:LYS:HD2	1.68	0.75
1:F:1:MET:CG	1:F:2:ASP:H	1.98	0.74
1:D:53:THR:HG22	1:F:7:LEU:HD21	1.70	0.74
1:B:69:GLN:HE22	1:B:122:HIS:HB2	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:H	1:D:117:ASN:ND2	1.86	0.73
1:C:33:GLN:HE21	1:C:33:GLN:H	1.38	0.72
1:A:82:GLN:HB2	1:A:163:ILE:HD13	1.71	0.72
1:A:137:LEU:HD13	1:A:215:LEU:HD22	1.71	0.71
1:C:198:ARG:HH12	1:C:202:GLU:HG2	1.55	0.71
1:D:1:MET:C	1:D:3:LYS:H	1.93	0.71
1:E:104:ILE:HG22	1:E:108:MET:HE1	1.72	0.70
1:B:17:ARG:O	1:B:21:GLU:HB3	1.92	0.70
1:C:14:TRP:HA	1:C:17:ARG:HE	1.57	0.70
1:C:33:GLN:H	1:C:33:GLN:NE2	1.89	0.70
1:E:1:MET:HE3	1:E:3:LYS:HD2	1.73	0.70
1:B:165:LYS:O	1:B:169:GLU:HG2	1.93	0.69
1:D:112:ASP:HA	1:D:117:ASN:HD21	1.58	0.68
1:C:185:ASP:HA	1:E:26:PHE:CD1	2.28	0.68
1:C:198:ARG:NH1	1:C:202:GLU:HG2	2.08	0.68
1:C:4:ILE:O	1:C:8:PHE:HB2	1.95	0.67
1:F:78:LEU:HD22	1:F:163:ILE:HD12	1.75	0.67
1:E:104:ILE:HG22	1:E:108:MET:CE	2.25	0.67
1:A:1:MET:HG3	1:A:3:LYS:H	1.59	0.67
1:B:14:TRP:O	1:B:18:MET:HG2	1.95	0.66
1:F:127:TRP:HD1	1:F:134:LEU:HD13	1.60	0.66
1:D:17:ARG:O	1:D:21:GLU:HB3	1.96	0.66
1:D:28:GLU:HA	1:D:31:ASP:OD2	1.94	0.66
1:E:205:TYR:O	1:E:209:ILE:HG12	1.96	0.66
1:E:56:GLU:HG3	1:E:57:PRO:HD2	1.79	0.65
1:A:132:HIS:CE1	1:A:136:LYS:HE3	2.32	0.65
1:A:139:PRO:HA	1:A:142:ARG:HD2	1.79	0.65
1:E:156:TYR:HA	1:E:201:LEU:HD11	1.78	0.64
1:D:1:MET:C	1:D:3:LYS:N	2.49	0.64
1:E:32:HIS:NE2	1:E:56:GLU:HG2	2.12	0.64
1:C:1:MET:HG2	1:E:92:HIS:HE2	1.62	0.64
1:E:82:GLN:HB2	1:E:163:ILE:HD13	1.80	0.64
1:D:113:LEU:N	1:D:117:ASN:HD21	1.95	0.63
1:A:202:GLU:O	1:A:206:ARG:HD3	1.99	0.63
1:E:181:TYR:HB3	1:E:188:LEU:HD23	1.80	0.63
1:C:53:THR:HG22	1:E:7:LEU:HD21	1.80	0.62
1:E:134:LEU:HA	1:E:137:LEU:HD13	1.81	0.62
1:A:78:LEU:CD1	1:A:163:ILE:HD12	2.29	0.62
1:D:208:ALA:O	1:D:212:LEU:HD23	2.00	0.62
1:F:127:TRP:CD1	1:F:134:LEU:HD13	2.35	0.62
1:E:90:ILE:HD12	1:E:92:HIS:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:SER:HB2	1:A:194:MET:HE3	1.82	0.61
1:E:1:MET:O	1:E:5:LYS:HE2	2.01	0.60
1:E:219:ASN:HD22	1:E:219:ASN:N	1.96	0.60
1:C:185:ASP:HA	1:E:26:PHE:CE1	2.37	0.59
1:B:198:ARG:NH1	1:B:202:GLU:HG2	2.17	0.59
1:C:202:GLU:O	1:C:206:ARG:HG3	2.02	0.59
1:E:90:ILE:HD12	1:E:92:HIS:N	2.18	0.59
1:A:78:LEU:HD12	1:A:163:ILE:CD1	2.31	0.59
1:A:82:GLN:HB2	1:A:163:ILE:CD1	2.32	0.59
1:C:56:GLU:OE1	1:C:59:GLU:HG3	2.03	0.59
1:E:41:GLY:O	1:E:64:ARG:HA	2.04	0.58
1:C:1:MET:HG3	1:C:3:LYS:H	1.66	0.58
1:B:198:ARG:HH12	1:B:202:GLU:HG2	1.69	0.58
1:C:16:GLN:C	1:C:18:MET:H	2.08	0.57
1:E:14:TRP:O	1:E:18:MET:HG2	2.04	0.57
1:B:37:TYR:HB2	1:B:60:LEU:HD23	1.87	0.57
1:C:35:PRO:HB3	1:C:59:GLU:O	2.05	0.57
1:A:208:ALA:O	1:A:212:LEU:HD23	2.04	0.56
1:D:69:GLN:NE2	1:D:123:ILE:HD11	2.19	0.56
1:D:112:ASP:HA	1:D:117:ASN:ND2	2.19	0.56
1:C:14:TRP:HA	1:C:17:ARG:NE	2.20	0.56
1:E:24:THR:O	1:E:28:GLU:HG3	2.05	0.56
1:F:1:MET:CE	1:F:3:LYS:H	2.14	0.56
1:C:206:ARG:HG2	1:C:206:ARG:HH11	1.69	0.56
1:B:5:LYS:H	1:B:5:LYS:HD2	1.69	0.56
1:E:219:ASN:N	1:E:219:ASN:ND2	2.54	0.56
1:B:133:LEU:HD23	1:B:133:LEU:C	2.26	0.56
1:B:213:SER:O	1:B:215:LEU:HG	2.05	0.56
1:E:99:THR:HG21	1:E:182:ASP:CG	2.26	0.56
1:C:12:TYR:O	1:C:16:GLN:HB2	2.06	0.56
1:C:53:THR:HB	1:C:55:LEU:HG	1.87	0.56
1:E:27:LYS:C	1:E:29:LEU:H	2.09	0.56
1:F:140:GLU:N	1:F:140:GLU:OE1	2.36	0.56
1:E:150:ASN:O	1:E:154:GLN:HG2	2.06	0.56
1:B:93:ILE:HG21	1:B:158:LEU:HD21	1.86	0.55
1:C:10:ASN:N	1:C:10:ASN:HD22	2.02	0.55
1:C:94:ILE:HD13	1:C:179:TRP:CH2	2.41	0.55
1:E:16:GLN:HE21	1:E:16:GLN:CA	2.14	0.55
1:E:198:ARG:NH1	4:E:5243:HOH:O	2.29	0.55
1:A:1:MET:HG3	1:A:2:ASP:H	1.70	0.55
1:E:99:THR:HG22	1:E:182:ASP:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ALA:O	1:E:212:LEU:HD23	2.06	0.55
1:E:202:GLU:O	1:E:206:ARG:HB2	2.07	0.55
1:D:113:LEU:N	1:D:117:ASN:ND2	2.55	0.55
1:B:150:ASN:O	1:B:154:GLN:HG2	2.07	0.54
1:C:46:ARG:HG3	1:C:183:VAL:HG11	1.89	0.54
1:C:137:LEU:HD23	1:C:142:ARG:HA	1.89	0.54
1:F:82:GLN:HB2	1:F:163:ILE:HD13	1.89	0.54
1:C:134:LEU:O	1:C:142:ARG:NH1	2.40	0.54
1:E:20:GLU:HG3	1:E:21:GLU:OE1	2.07	0.54
1:E:159:GLY:HA3	1:E:201:LEU:HD22	1.90	0.53
1:A:16:GLN:O	1:A:20:GLU:HG2	2.07	0.53
1:C:29:LEU:HD13	1:C:29:LEU:C	2.29	0.53
1:A:16:GLN:OE1	1:A:16:GLN:HA	2.07	0.53
1:E:161:THR:HG22	4:F:6253:HOH:O	2.08	0.52
1:A:1:MET:CG	1:A:2:ASP:N	2.72	0.52
1:A:5:LYS:O	1:A:5:LYS:HD3	2.10	0.52
1:E:16:GLN:HA	1:E:16:GLN:NE2	2.19	0.52
1:F:133:LEU:C	1:F:133:LEU:HD23	2.30	0.52
1:B:133:LEU:HD21	1:B:145:MET:HE3	1.91	0.52
1:A:1:MET:HG3	1:A:3:LYS:N	2.25	0.52
1:C:193:VAL:HA	1:C:204:SER:OG	2.09	0.52
1:D:198:ARG:NH1	4:D:4259:HOH:O	2.43	0.52
1:E:16:GLN:O	1:E:20:GLU:HG2	2.09	0.52
1:C:37:TYR:HB2	1:C:60:LEU:HD23	1.90	0.52
1:C:46:ARG:HG3	1:C:183:VAL:CG1	2.40	0.52
1:E:130:HIS:CD2	1:E:149:ILE:HG21	2.45	0.52
1:E:133:LEU:C	1:E:133:LEU:HD23	2.30	0.52
1:D:37:TYR:OH	1:F:3:LYS:HB3	2.09	0.52
1:A:185:ASP:OD1	1:A:187:PHE:HD1	1.94	0.51
1:B:133:LEU:O	1:B:136:LYS:HG2	2.09	0.51
1:B:217:GLU:OE2	1:B:220:ILE:HD12	2.10	0.51
1:C:133:LEU:C	1:C:133:LEU:HD23	2.30	0.51
1:B:41:GLY:O	1:B:64:ARG:HA	2.11	0.51
1:E:185:ASP:HB3	1:E:187:PHE:HD1	1.76	0.51
1:E:1:MET:O	1:E:5:LYS:HG3	2.11	0.51
1:B:193:VAL:HA	1:B:204:SER:OG	2.10	0.51
1:C:138:SER:HB2	1:C:219:ASN:HB2	1.92	0.50
1:C:206:ARG:HG2	1:C:206:ARG:NH1	2.26	0.50
1:C:135:GLY:HA2	1:C:142:ARG:HH12	1.75	0.50
1:C:208:ALA:O	1:C:212:LEU:HG	2.11	0.50
1:E:98:HIS:HE1	1:E:101:CYS:HA	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HG	1:C:138:SER:H	1.75	0.50
1:F:37:TYR:HB2	1:F:60:LEU:HD23	1.94	0.50
1:C:200:THR:O	1:C:204:SER:HB3	2.11	0.50
1:B:104:ILE:O	1:B:108:MET:HG3	2.12	0.50
1:C:198:ARG:HH12	1:C:202:GLU:CG	2.25	0.50
1:D:14:TRP:O	1:D:18:MET:HG2	2.12	0.50
1:C:138:SER:HB2	1:C:219:ASN:CB	2.42	0.49
1:A:66:VAL:O	1:A:67:ALA:HB3	2.13	0.49
1:E:6:GLN:O	1:E:9:ALA:HB3	2.12	0.49
1:F:24:THR:O	1:F:28:GLU:HG3	2.11	0.49
1:A:3:LYS:O	1:A:7:LEU:HD13	2.13	0.49
1:C:16:GLN:O	1:C:20:GLU:HG2	2.12	0.49
1:D:166:SER:O	1:D:170:ARG:HG2	2.12	0.49
1:E:93:ILE:HG21	1:E:158:LEU:HD21	1.95	0.48
1:A:46:ARG:HG3	1:A:183:VAL:HG11	1.94	0.48
1:C:187:PHE:CE1	1:E:15:ALA:HB1	2.47	0.48
1:E:198:ARG:HD2	1:E:198:ARG:O	2.13	0.48
1:C:82:GLN:NE2	1:C:86:ASP:HB2	2.28	0.48
1:C:98:HIS:HE1	1:C:101:CYS:HA	1.78	0.48
1:D:82:GLN:HB2	1:D:163:ILE:CD1	2.40	0.48
1:E:151:VAL:HG21	1:E:180:VAL:HG22	1.95	0.48
1:D:69:GLN:NE2	1:D:123:ILE:CD1	2.77	0.48
1:C:218:GLU:O	1:C:219:ASN:C	2.52	0.48
1:D:93:ILE:HG21	1:D:158:LEU:HD21	1.95	0.48
1:E:127:TRP:HD1	1:E:134:LEU:HD13	1.79	0.48
1:C:10:ASN:N	1:C:10:ASN:ND2	2.62	0.48
1:C:19:LYS:C	1:C:21:GLU:H	2.17	0.48
1:C:48:PRO:CG	1:E:50:GLU:HG2	2.44	0.47
1:D:66:VAL:O	1:D:67:ALA:HB3	2.14	0.47
1:E:137:LEU:HD21	1:E:145:MET:HE2	1.96	0.47
1:F:20:GLU:C	1:F:22:ASN:H	2.17	0.47
1:D:22:ASN:C	1:D:22:ASN:HD22	2.16	0.47
1:B:50:GLU:H	1:B:50:GLU:CD	2.17	0.47
1:F:127:TRP:HD1	1:F:134:LEU:CD1	2.24	0.47
1:F:166:SER:O	1:F:170:ARG:HG2	2.14	0.47
1:C:18:MET:HG2	1:C:26:PHE:CE1	2.49	0.47
1:D:126:ILE:HG23	1:D:153:GLU:HG3	1.96	0.47
1:E:90:ILE:CD1	1:E:92:HIS:O	2.63	0.47
1:F:14:TRP:O	1:F:18:MET:HG2	2.14	0.47
1:C:18:MET:HG2	1:C:26:PHE:HE1	1.80	0.47
1:C:52:LEU:HD11	1:C:181:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:GLU:O	1:E:203:ILE:HG13	2.14	0.47
1:F:112:ASP:HB3	4:F:6258:HOH:O	2.14	0.47
1:E:140:GLU:OE1	1:E:140:GLU:N	2.41	0.47
1:E:193:VAL:HA	1:E:204:SER:HB2	1.97	0.47
1:E:165:LYS:HE2	1:E:198:ARG:NH1	2.30	0.47
1:E:181:TYR:CD1	1:E:181:TYR:C	2.87	0.47
1:F:133:LEU:HD23	1:F:133:LEU:O	2.15	0.47
1:D:32:HIS:HD2	1:D:59:GLU:OE1	1.98	0.46
1:A:24:THR:O	1:A:28:GLU:HG3	2.14	0.46
1:B:2:ASP:HB3	1:B:3:LYS:H	1.54	0.46
1:F:52:LEU:HD11	1:F:181:TYR:CE2	2.50	0.46
1:D:150:ASN:O	1:D:154:GLN:HG2	2.15	0.46
1:F:1:MET:HE1	1:F:3:LYS:HG3	1.98	0.46
1:C:10:ASN:ND2	1:C:10:ASN:H	2.13	0.46
1:D:16:GLN:O	1:D:20:GLU:HG2	2.16	0.46
1:E:137:LEU:HD11	1:E:215:LEU:HD21	1.96	0.46
1:F:1:MET:CG	1:F:2:ASP:N	2.69	0.46
1:D:1:MET:O	1:D:3:LYS:N	2.49	0.46
1:F:175:SER:HA	1:F:195:ALA:O	2.15	0.46
1:F:198:ARG:HH11	1:F:202:GLU:HG2	1.77	0.46
1:B:181:TYR:HB3	1:B:188:LEU:HD23	1.97	0.46
1:C:53:THR:CB	1:C:55:LEU:HG	2.46	0.46
1:A:160:ARG:HG2	1:A:198:ARG:HH12	1.80	0.45
1:D:22:ASN:C	1:D:22:ASN:ND2	2.69	0.45
1:C:66:VAL:O	1:C:67:ALA:HB3	2.16	0.45
1:F:91:GLU:HG2	1:F:173:LYS:O	2.17	0.45
1:F:156:TYR:O	1:F:160:ARG:HD3	2.16	0.45
1:C:112:ASP:HA	1:C:117:ASN:ND2	2.31	0.45
1:E:62:VAL:HG12	1:E:63:HIS:N	2.31	0.45
1:D:83:TYR:O	1:D:87:VAL:HB	2.17	0.45
1:A:182:ASP:C	1:A:184:ASN:H	2.21	0.45
1:E:16:GLN:C	1:E:18:MET:H	2.19	0.45
1:C:28:GLU:O	1:C:31:ASP:HB2	2.16	0.44
1:C:150:ASN:O	1:C:154:GLN:HG2	2.17	0.44
1:D:91:GLU:HG2	1:D:173:LYS:O	2.18	0.44
1:F:78:LEU:HD23	1:F:78:LEU:HA	1.89	0.44
1:C:4:ILE:HD11	1:E:92:HIS:ND1	2.33	0.44
1:D:54:ASN:C	1:D:54:ASN:HD22	2.20	0.44
1:E:99:THR:HG23	1:E:183:VAL:HG22	2.00	0.44
1:D:7:LEU:HD21	1:F:53:THR:HG22	2.00	0.44
1:F:198:ARG:HH12	1:F:202:GLU:HG2	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:HD3	4:D:4260:HOH:O	2.17	0.44
1:D:175:SER:HA	1:D:195:ALA:O	2.18	0.44
1:D:21:GLU:O	1:D:21:GLU:HG2	2.18	0.44
1:F:195:ALA:HB2	1:F:201:LEU:HA	1.98	0.44
1:B:216:ASP:O	1:B:220:ILE:HG13	2.17	0.44
1:C:175:SER:HA	1:C:195:ALA:O	2.18	0.44
1:D:37:TYR:HB2	1:D:60:LEU:HD23	2.00	0.44
1:C:84:ALA:HB1	1:C:90:ILE:HD12	1.99	0.43
1:D:17:ARG:HH11	1:D:17:ARG:HB3	1.83	0.43
1:E:46:ARG:HB2	1:E:181:TYR:OH	2.18	0.43
1:E:50:GLU:CD	1:E:50:GLU:H	2.21	0.43
1:E:136:LYS:O	1:E:220:ILE:HG13	2.18	0.43
1:F:16:GLN:O	1:F:19:LYS:HB3	2.18	0.43
1:A:1:MET:CG	1:A:2:ASP:H	2.31	0.43
1:B:66:VAL:O	1:B:67:ALA:HB3	2.18	0.43
1:D:1:MET:SD	1:F:92:HIS:NE2	2.90	0.43
1:D:6:GLN:O	1:D:10:ASN:OD1	2.37	0.43
1:C:140:GLU:OE2	1:C:141:LYS:HG2	2.19	0.43
1:D:55:LEU:CD1	1:D:60:LEU:HD21	2.48	0.43
1:B:166:SER:O	1:B:170:ARG:HG2	2.18	0.43
1:C:1:MET:HG2	1:E:92:HIS:NE2	2.31	0.43
1:D:2:ASP:HA	1:D:5:LYS:NZ	2.33	0.43
1:F:66:VAL:O	1:F:67:ALA:HB3	2.17	0.43
1:F:139:PRO:HA	1:F:142:ARG:HD2	2.00	0.43
1:B:127:TRP:CD1	1:B:134:LEU:HD13	2.54	0.43
1:E:53:THR:OG1	1:E:55:LEU:HG	2.19	0.43
1:B:5:LYS:N	1:B:5:LYS:HE3	2.34	0.43
1:D:12:TYR:O	1:D:16:GLN:HB2	2.19	0.43
1:C:94:ILE:HD13	1:C:179:TRP:CZ3	2.54	0.43
1:C:104:ILE:O	1:C:108:MET:HG3	2.19	0.43
1:D:4:ILE:O	1:D:7:LEU:HB3	2.19	0.43
1:D:198:ARG:HA	1:D:198:ARG:HD2	1.81	0.43
3:E:1006:SO4:O4	1:F:124:ARG:HD3	2.18	0.43
1:A:56:GLU:OE1	1:A:59:GLU:HG3	2.20	0.42
1:C:7:LEU:C	1:C:7:LEU:HD23	2.39	0.42
1:D:46:ARG:NH2	1:F:29:LEU:HD22	2.34	0.42
1:D:50:GLU:HG2	1:F:48:PRO:HG2	2.01	0.42
1:A:23:SER:C	1:A:25:TYR:H	2.22	0.42
1:C:16:GLN:O	1:C:18:MET:N	2.50	0.42
1:C:34:THR:HA	1:C:35:PRO:HD3	1.86	0.42
1:E:127:TRP:CD1	1:E:134:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HA	1:A:35:PRO:HD3	1.80	0.42
1:A:216:ASP:O	1:A:220:ILE:HG13	2.19	0.42
1:F:112:ASP:HA	1:F:117:ASN:HD21	1.84	0.42
1:A:195:ALA:HB2	1:A:201:LEU:HA	2.01	0.42
1:E:29:LEU:C	1:E:29:LEU:HD23	2.39	0.42
1:C:1:MET:HB3	1:E:92:HIS:CE1	2.55	0.42
1:E:194:MET:O	1:E:194:MET:SD	2.78	0.42
1:E:195:ALA:HB2	1:E:201:LEU:HA	2.01	0.42
1:A:208:ALA:O	1:A:212:LEU:CD2	2.68	0.42
1:B:82:GLN:HB2	1:B:163:ILE:HD13	2.02	0.42
1:D:7:LEU:HD13	1:F:179:TRP:HH2	1.85	0.42
1:E:108:MET:CE	1:E:143:ALA:HA	2.50	0.42
1:B:2:ASP:O	1:B:4:ILE:N	2.54	0.41
1:C:48:PRO:HG3	1:E:50:GLU:HG2	2.01	0.41
1:E:137:LEU:HD21	1:E:145:MET:CE	2.50	0.41
1:F:161:THR:O	1:F:165:LYS:HG3	2.20	0.41
1:B:2:ASP:O	1:B:5:LYS:HD2	2.21	0.41
1:D:1:MET:CG	1:F:173:LYS:HZ1	2.33	0.41
1:A:150:ASN:O	1:A:154:GLN:HG2	2.21	0.41
1:B:176:LEU:O	1:B:194:MET:HA	2.21	0.41
1:D:185:ASP:OD1	1:D:187:PHE:HD1	2.02	0.41
1:F:135:GLY:C	1:F:137:LEU:H	2.23	0.41
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.85	0.41
1:B:83:TYR:O	1:B:87:VAL:HB	2.20	0.41
1:C:99:THR:OG1	1:C:183:VAL:HG22	2.20	0.41
1:C:166:SER:O	1:C:170:ARG:HG2	2.20	0.41
1:F:20:GLU:C	1:F:22:ASN:N	2.74	0.41
1:E:82:GLN:HB2	1:E:163:ILE:CD1	2.50	0.41
1:F:34:THR:HA	1:F:35:PRO:HD3	1.80	0.41
1:E:25:TYR:HD2	1:E:26:PHE:CE2	2.38	0.41
1:E:99:THR:HG22	1:E:183:VAL:H	1.85	0.41
1:C:18:MET:HG3	1:C:23:SER:HB3	2.01	0.41
1:A:206:ARG:HG2	1:A:206:ARG:NH1	2.35	0.40
1:E:71:ILE:HD13	1:E:122:HIS:CD2	2.57	0.40
1:E:193:VAL:HG22	1:E:205:TYR:HA	2.03	0.40
1:B:5:LYS:H	1:B:5:LYS:CD	2.33	0.40
1:B:130:HIS:CD2	1:B:149:ILE:HG21	2.56	0.40
1:C:8:PHE:HE1	1:E:188:LEU:O	2.03	0.40
1:C:33:GLN:NE2	1:C:33:GLN:N	2.65	0.40
1:C:198:ARG:NH1	1:C:201:LEU:HD23	2.36	0.40
1:A:78:LEU:HA	1:A:78:LEU:HD13	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:HE1	1:A:195:ALA:C	2.41	0.40
1:C:62:VAL:HG12	1:C:63:HIS:N	2.36	0.40
1:D:5:LYS:H	1:D:5:LYS:HG3	1.69	0.40
1:D:190:ASP:OD1	1:D:191:GLN:N	2.54	0.40
1:F:1:MET:CE	1:F:2:ASP:HB3	2.51	0.40
1:F:181:TYR:HB3	1:F:188:LEU:HD23	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	219/229 (96%)	202 (92%)	14 (6%)	3 (1%)	11	11
1	B	219/229 (96%)	200 (91%)	16 (7%)	3 (1%)	11	11
1	C	217/229 (95%)	191 (88%)	22 (10%)	4 (2%)	8	7
1	D	213/229 (93%)	201 (94%)	11 (5%)	1 (0%)	29	35
1	E	218/229 (95%)	194 (89%)	23 (11%)	1 (0%)	29	35
1	F	217/229 (95%)	204 (94%)	12 (6%)	1 (0%)	29	35
All	All	1303/1374 (95%)	1192 (92%)	98 (8%)	13 (1%)	15	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASP
1	B	3	LYS
1	B	22	ASN
1	C	25	TYR
1	A	22	ASN
1	A	140	GLU

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Mol	Chain	Res	Type
1	C	24	THR
1	E	46	ARG
1	C	17	ARG
1	F	21	GLU
1	D	19	LYS
1	A	183	VAL
1	C	55	LEU

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	193/201 (96%)	188 (97%)	5 (3%)	46	63
1	B	193/201 (96%)	184 (95%)	9 (5%)	26	37
1	C	191/201 (95%)	183 (96%)	8 (4%)	30	42
1	D	187/201 (93%)	182 (97%)	5 (3%)	44	61
1	E	192/201 (96%)	180 (94%)	12 (6%)	18	24
1	F	191/201 (95%)	187 (98%)	4 (2%)	53	70
All	All	1147/1206 (95%)	1104 (96%)	43 (4%)	34	48

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	54	ASN
1	A	78	LEU
1	A	194	MET
1	A	206	ARG
1	B	1	MET
1	B	2	ASP
1	B	5	LYS
1	B	29	LEU
1	B	33	GLN
1	B	54	ASN

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Mol	Chain	Res	Type
1	B	68	ASN
1	B	78	LEU
1	B	140	GLU
1	C	8	PHE
1	C	18	MET
1	C	33	GLN
1	C	54	ASN
1	C	68	ASN
1	C	75	PHE
1	C	140	GLU
1	C	145	MET
1	D	22	ASN
1	D	54	ASN
1	D	75	PHE
1	D	137	LEU
1	D	169	GLU
1	E	1	MET
1	E	8	PHE
1	E	16	GLN
1	E	21	GLU
1	E	54	ASN
1	E	78	LEU
1	E	90	ILE
1	E	132	HIS
1	E	194	MET
1	E	206	ARG
1	E	217	GLU
1	E	219	ASN
1	F	21	GLU
1	F	29	LEU
1	F	194	MET
1	F	198	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	132	HIS
1	A	219	ASN
1	B	54	ASN
1	B	69	GLN
1	C	6	GLN

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Mol	Chain	Res	Type
1	C	10	ASN
1	C	33	GLN
1	C	54	ASN
1	C	219	ASN
1	D	16	GLN
1	D	22	ASN
1	D	54	ASN
1	D	69	GLN
1	D	100	ASN
1	D	117	ASN
1	E	16	GLN
1	E	22	ASN
1	E	33	GLN
1	E	54	ASN
1	E	219	ASN
1	F	54	ASN
1	F	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\lvert Z \rvert > 2$	Counts	RMSZ	$\#\lvert Z \rvert > 2$
3	SO4	B	1001	-	4,4,4	0.24	0	6,6,6	0.23	0
3	SO4	B	1002	-	4,4,4	0.22	0	6,6,6	0.23	0
3	SO4	D	1004	-	4,4,4	0.29	0	6,6,6	0.12	0
3	SO4	E	1006	-	4,4,4	0.27	0	6,6,6	0.06	0
3	SO4	E	1005	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	D	1003	-	4,4,4	0.25	0	6,6,6	0.06	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1006	SO4	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(Å²)	Q<0.9
1	A	221/229 (96%)	0.48	28 (12%)	3	5	28, 47, 97, 100	0
1	B	221/229 (96%)	0.47	27 (12%)	4	6	27, 53, 95, 100	0
1	C	219/229 (95%)	0.68	28 (12%)	3	5	33, 58, 99, 100	0
1	D	215/229 (93%)	0.38	16 (7%)	14	19	31, 50, 92, 100	0
1	E	220/229 (96%)	0.88	39 (17%)	1	1	34, 68, 96, 100	0
1	F	219/229 (95%)	0.55	29 (13%)	3	4	31, 57, 88, 100	0
All	All	1315/1374 (95%)	0.58	167 (12%)	3	5	27, 55, 95, 100	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	GLU	6.8
1	E	24	THR	6.1
1	A	20	GLU	6.0
1	E	20	GLU	5.5
1	E	27	LYS	5.4
1	E	40	ILE	5.3
1	C	22	ASN	5.1
1	C	7	LEU	4.9
1	F	217	GLU	4.7
1	A	29	LEU	4.7
1	A	32	HIS	4.6
1	D	23	SER	4.5
1	A	25	TYR	4.5
1	C	2	ASP	4.4
1	A	27	LYS	4.4
1	C	12	TYR	4.4
1	C	19	LYS	4.3
1	E	187	PHE	4.2
1	B	20	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	31	ASP	4.0
1	A	19	LYS	4.0
1	D	20	GLU	4.0
1	F	218	GLU	4.0
1	A	1	MET	3.9
1	B	28	GLU	3.9
1	F	31	ASP	3.8
1	F	40	ILE	3.8
1	A	24	THR	3.8
1	E	23	SER	3.8
1	A	22	ASN	3.7
1	B	24	THR	3.7
1	D	1	MET	3.7
1	B	40	ILE	3.7
1	F	215	LEU	3.7
1	A	31	ASP	3.7
1	B	22	ASN	3.7
1	A	23	SER	3.7
1	F	216	ASP	3.6
1	E	32	HIS	3.6
1	C	24	THR	3.6
1	E	132	HIS	3.5
1	B	2	ASP	3.5
1	E	136	LYS	3.5
1	B	221	LEU	3.5
1	B	219	ASN	3.5
1	B	220	ILE	3.5
1	C	93	ILE	3.4
1	E	38	LEU	3.4
1	A	40	ILE	3.4
1	E	95	ILE	3.4
1	E	22	ASN	3.4
1	C	1	MET	3.4
1	D	2	ASP	3.3
1	E	183	VAL	3.3
1	C	14	TRP	3.3
1	C	6	GLN	3.3
1	C	40	ILE	3.3
1	F	24	THR	3.3
1	C	217	GLU	3.2
1	A	62	VAL	3.2
1	F	136	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	33	GLN	3.1
1	E	93	ILE	3.1
1	E	219	ASN	3.1
1	C	132	HIS	3.1
1	F	62	VAL	3.1
1	E	1	MET	3.1
1	E	217	GLU	3.1
1	F	38	LEU	3.0
1	D	27	LYS	3.0
1	E	12	TYR	3.0
1	B	132	HIS	3.0
1	A	28	GLU	2.9
1	E	41	GLY	2.9
1	F	93	ILE	2.9
1	F	28	GLU	2.9
1	F	95	ILE	2.9
1	B	32	HIS	2.9
1	E	2	ASP	2.9
1	C	5	LYS	2.9
1	B	31	ASP	2.9
1	B	25	TYR	2.8
1	B	1	MET	2.8
1	F	1	MET	2.8
1	B	29	LEU	2.8
1	C	38	LEU	2.8
1	E	33	GLN	2.8
1	F	176	LEU	2.8
1	E	28	GLU	2.8
1	E	21	GLU	2.7
1	F	94	ILE	2.7
1	C	31	ASP	2.7
1	F	30	ALA	2.7
1	D	22	ASN	2.7
1	D	132	HIS	2.7
1	D	12	TYR	2.7
1	B	96	CYS	2.7
1	C	28	GLU	2.7
1	D	19	LYS	2.7
1	F	155	VAL	2.6
1	F	132	HIS	2.6
1	A	183	VAL	2.6
1	B	38	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	62	VAL	2.6
1	F	22	ASN	2.6
1	A	33	GLN	2.6
1	E	218	GLU	2.5
1	B	218	GLU	2.5
1	B	62	VAL	2.5
1	D	70	VAL	2.5
1	F	110	ASP	2.5
1	D	110	ASP	2.4
1	F	138	SER	2.4
1	E	137	LEU	2.4
1	B	41	GLY	2.4
1	B	39	TRP	2.4
1	A	26	PHE	2.4
1	B	27	LYS	2.4
1	D	40	ILE	2.4
1	E	94	ILE	2.4
1	A	158	LEU	2.4
1	D	21	GLU	2.4
1	F	33	GLN	2.4
1	A	41	GLY	2.4
1	A	70	VAL	2.4
1	F	20	GLU	2.4
1	F	27	LYS	2.3
1	B	19	LYS	2.3
1	C	113	LEU	2.3
1	C	18	MET	2.3
1	C	187	PHE	2.3
1	A	93	ILE	2.3
1	C	111	LYS	2.3
1	C	23	SER	2.3
1	A	169	GLU	2.3
1	A	95	ILE	2.3
1	A	132	HIS	2.2
1	A	217	GLU	2.2
1	E	176	LEU	2.2
1	C	3	LYS	2.2
1	E	97	GLY	2.2
1	E	215	LEU	2.2
1	E	138	SER	2.2
1	F	39	TRP	2.2
1	C	62	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	17	ARG	2.2
1	F	151	VAL	2.1
1	B	42	CYS	2.1
1	E	39	TRP	2.1
1	B	217	GLU	2.1
1	C	81	VAL	2.1
1	E	128	PHE	2.1
1	A	2	ASP	2.1
1	E	220	ILE	2.1
1	D	214	ILE	2.1
1	E	26	PHE	2.1
1	B	95	ILE	2.1
1	A	110	ASP	2.1
1	C	27	LYS	2.1
1	E	135	GLY	2.1
1	F	60	LEU	2.0
1	B	21	GLU	2.0
1	E	56	GLU	2.0
1	E	19	LYS	2.0
1	E	151	VAL	2.0
1	A	39	TRP	2.0
1	F	61	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	E	1005	5/5	0.93	0.17	98,98,99,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	1004	5/5	0.94	0.14	77,80,81,81	0
3	SO4	E	1006	5/5	0.94	0.14	90,92,92,93	0
3	SO4	B	1002	5/5	0.95	0.17	59,63,64,64	0
3	SO4	B	1001	5/5	0.96	0.13	65,67,69,69	0
3	SO4	D	1003	5/5	0.97	0.11	91,92,92,93	0
2	ZN	C	3230	1/1	0.99	0.09	53,53,53,53	0
2	ZN	D	4230	1/1	0.99	0.09	42,42,42,42	0
2	ZN	E	5230	1/1	0.99	0.07	57,57,57,57	0
2	ZN	F	6230	1/1	0.99	0.10	50,50,50,50	0
2	ZN	B	2230	1/1	0.99	0.10	44,44,44,44	0
2	ZN	A	1230	1/1	1.00	0.12	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.