WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2022 – 06:09 PM JST

PDB ID	:	6IVW
Title	:	Crystal structure of a bacterial Bestrophin homolog from Klebsiella pneumoniae with a mutation D269A
Authors	:	Kittredge, A.; Chen, S.; Yang, T.
Deposited on	:	2018-12-04
Resolution	:	3.72 Å(reported)

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

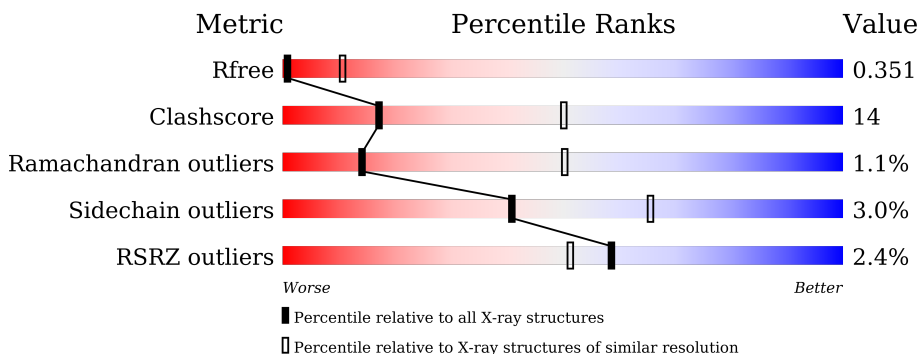|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.72 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		0.351
Clashscore		14
Ramachandran outliers		1.1%
Sidechain outliers		3.0%
RSRZ outliers		2.4%

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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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 <=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	296	4% — 60% / 29% / • / 9%
1	B	296	% — 61% / 26% / • / 10%
1	C	296	3% — 62% / 26% / • / 10%
1	D	296	61% / 28% / • / 9%
1	E	296	2% — 56% / 33% / • / 9%

WORLDWIDE PDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10562 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 Bestrophin homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2117	1372	359	377	9			
1	B	266	Total	C	N	O	S	0	0	0
			2100	1364	353	375	8			
1	C	265	Total	C	N	O	S	0	0	0
			2076	1342	355	370	9			
1	D	268	Total	C	N	O	S	0	0	0
			2111	1366	359	377	9			
1	E	270	Total	C	N	O	S	0	0	0
			2149	1395	364	381	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP W1ELP7
A	0	ALA	-	expression tag	UNP W1ELP7
A	269	ALA	ASP	engineered mutation	UNP W1ELP7
B	-1	ASN	-	expression tag	UNP W1ELP7
B	0	ALA	-	expression tag	UNP W1ELP7
B	269	ALA	ASP	engineered mutation	UNP W1ELP7
C	-1	ASN	-	expression tag	UNP W1ELP7
C	0	ALA	-	expression tag	UNP W1ELP7
C	269	ALA	ASP	engineered mutation	UNP W1ELP7
D	-1	ASN	-	expression tag	UNP W1ELP7
D	0	ALA	-	expression tag	UNP W1ELP7
D	269	ALA	ASP	engineered mutation	UNP W1ELP7
E	-1	ASN	-	expression tag	UNP W1ELP7
E	0	ALA	-	expression tag	UNP W1ELP7
E	269	ALA	ASP	engineered mutation	UNP W1ELP7

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

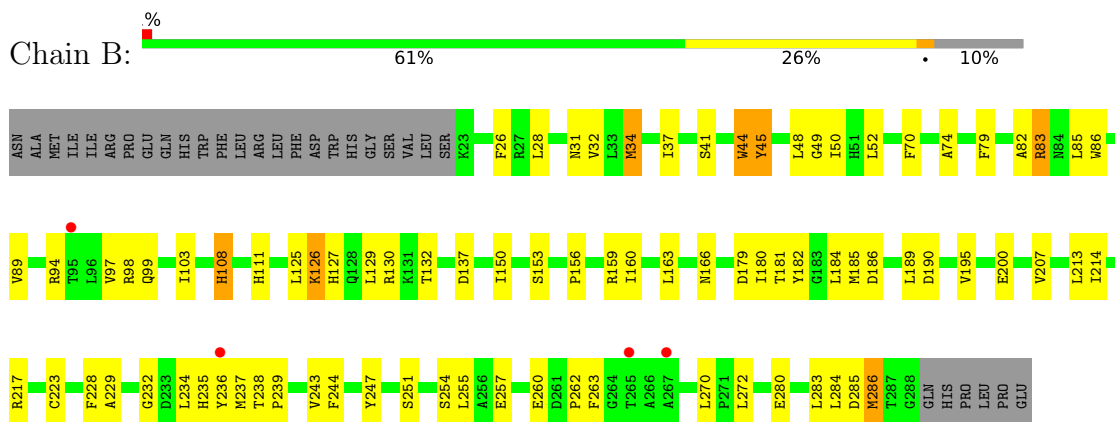| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Zn 3	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0

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.
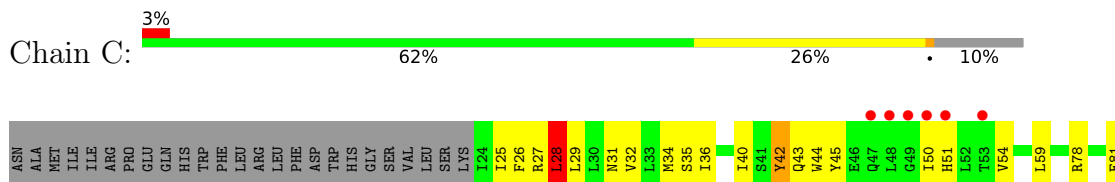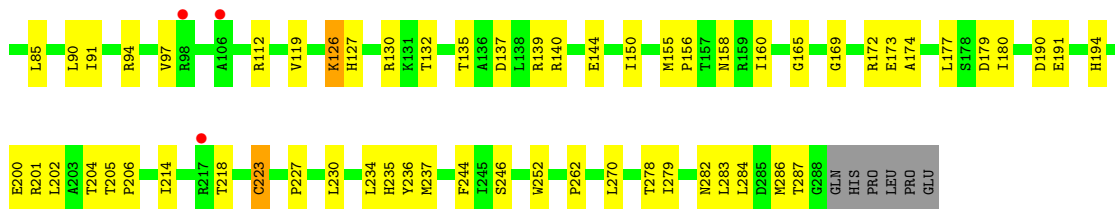
• Molecule 1: Bestrophin homolog

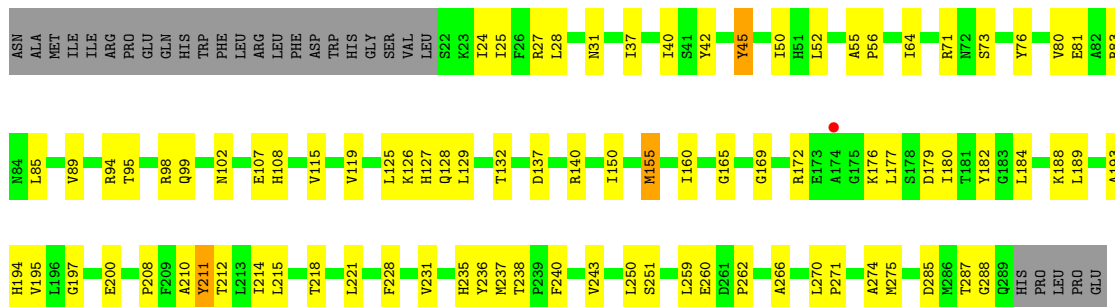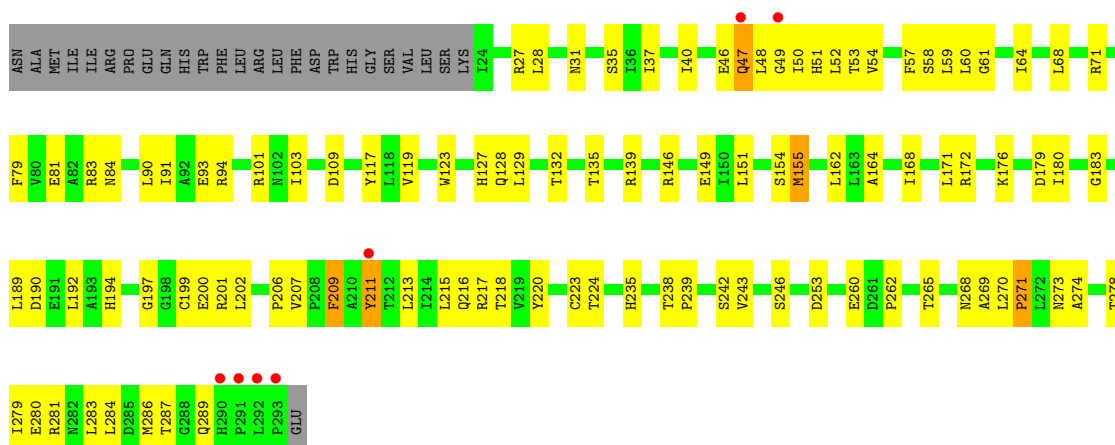• Molecule 1: Bestrophin homolog

• Molecule 1: Bestrophin homolog

L85 L90 I91 R94 V97 R98 A106 R112 V119 K126 H127 R130 K131 T132 T135 A136 D137 L138 R139 R140 E444 I150 M155 P156 T157 N158 R159 I160 G165 G169 R172 E173 A174 L177 S178 D179 I180 D190 E191 H194

E200 R201 L202 A203 T204 T205 P206 I214 R217 T218 C223 P227 L230 L234 H235 Y236 M237 F244 I245 S246 W252 P262 L270 T278 I279 N282 L283 L284 D285 M286 T287 G288 GLN HIS PRO LEU GLU

• Molecule 1: Bestrophin homolog

Chain D:

61%   28%   •   9%

ASN ALA MET ILE ILE ARG PRO GLU GLN HIS TRP PHE LEU ARG LEU PHE ASP TRP HIS GLY SER VAL LEU S22 K23 I24 I25 F26 R27 L28 N31 I37 I40 S41 Y42 Y45 I50 H51 L52 A55 P56 I64 R71 N72 S73 Y76 V80 E81 A82 R83

N84 L85 V89 R94 T95 R98 Q99 N102 E107 H108 V115 V119 L125 K126 H127 Q128 L129 T132 D137 R140 I150 M155 I160 G165 G169 R172 E173 A174 G175 K176 L177 S178 D179 I180 T181 Y182 G183 L184 K188 L189 A193

H194 V195 L196 G197 E200 P208 F209 A210 Y211 T212 L213 I214 L215 T218 L221 F228 V231 H235 Y236 M237 T238 P239 F240 V243 L250 S251 L259 E260 D261 P262 A266 L270 P271 A274 M275 D285 M286 T287 Q288 G288 HIS PRO LEU GLU

• Molecule 1: Bestrophin homolog

Chain E:

2%   56%   33%   •   9%

ASN ALA MET ILE ILE ARG PRO GLU GLN HIS TRP PHE LEU ARG LEU PHE ASP TRP HIS GLY SER VAL LEU SER LYS I24 R27 L28 N31 S35 I36 I37 I40 E46 Q47 L48 G49 I50 H51 L52 T53 V54 F57 S58 L59 L60 G61 I64 L68 R71

F79 V80 E81 A82 R83 N84 L90 I91 A92 E93 R94 R101 N102 I103 D109 Y117 L118 V119 W123 H127 Q128 L129 T132 T135 R139 R146 E149 I150 L151 S154 M155 L162 L163 A164 I168 L171 R172 K176 D179 I180 G183

L189 D190 E191 L192 A193 H194 G197 G198 C199 E200 R201 L202 P206 V207 P208 F209 A210 Y211 T212 L213 I214 L215 Q216 R217 T218 V219 Y220 C223 T224 H235 T238 P239 S242 V243 S246 D253 E260 D261 P262 T265 N268 A269 L270 P271 L272 N273 A274 T278

I279 E280 R281 N282 L283 L284 D285 M286 T287 G288 Q288 H290 P291 L292 P293 GLU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.97Å 161.77Å 162.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.19 – 3.72 81.19 – 3.72	Depositor EDS
% Data completeness (in resolution range)	81.3 (81.19-3.72) 81.3 (81.19-3.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.289 , 0.351 0.289 , 0.351	Depositor DCC
R_{free} test set	1986 reflections (7.58%)	wwPDB-VP
Wilson B-factor (Å^2)	117.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 51.6	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10562	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

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	0.29	0/2163	0.49	0/2946
1	B	0.29	0/2146	0.51	0/2925
1	C	0.29	0/2119	0.49	0/2887
1	D	0.29	0/2156	0.51	0/2937
1	E	0.28	0/2198	0.51	0/2995
All	All	0.29	0/10782	0.50	0/14690

There are no bond length outliers.

There are no bond angle outliers.

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	2117	0	2152	81	0
1	B	2100	0	2134	68	0
1	C	2076	0	2111	58	0
1	D	2111	0	2145	68	0
1	E	2149	0	2196	86	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	2	0	0	0	0
All	All	10562	0	10738	297	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 14.

All (297) 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:A:98:ARG:NH2	1:E:190:ASP:OD1	2.13	0.81
1:D:231:VAL:HG12	1:D:238:THR:OG1	1.79	0.81
1:D:42:TYR:OH	1:D:228:PHE:O	2.00	0.78
1:C:139:ARG:NH1	1:C:144:GLU:OE1	2.17	0.77
1:B:34:MET:SD	1:B:34:MET:N	2.57	0.76
1:B:50:ILE:HB	1:D:237:MET:HG2	1.66	0.76
1:D:235:HIS:HD1	1:D:236:TYR:HD1	1.34	0.76
1:E:155:MET:SD	1:E:155:MET:N	2.60	0.75
1:D:177:LEU:HD13	1:D:182:TYR:HB2	1.69	0.74
1:C:155:MET:SD	1:E:94:ARG:NH2	2.62	0.72
1:B:186:ASP:OD2	1:D:99:GLN:NE2	2.22	0.72
1:B:130:ARG:NH2	1:B:270:LEU:O	2.23	0.70
1:E:207:VAL:O	1:E:209:PHE:N	2.25	0.69
1:A:101:ARG:NH2	1:A:286:MET:O	2.25	0.69
1:C:31:ASN:ND2	1:C:246:SER:OG	2.26	0.69
1:B:180:ILE:HG13	1:D:180:ILE:HD12	1.74	0.69
1:C:54:VAL:HG21	1:D:55:ALA:HB1	1.73	0.68
1:E:68:LEU:HD23	1:E:215:LEU:HD13	1.75	0.68
1:A:81:GLU:OE2	1:A:201:ARG:NH1	2.26	0.68
1:A:200:GLU:O	1:A:204:THR:OG1	2.11	0.67
1:A:270:LEU:HD22	1:A:275:MET:HE1	1.78	0.66
1:D:31:ASN:HD21	1:D:243:VAL:HA	1.60	0.65
1:B:150:ILE:HD13	1:B:160:ILE:HG12	1.78	0.65
1:C:278:THR:O	1:C:282:ASN:ND2	2.28	0.65
1:E:172:ARG:NH2	1:E:179:ASP:OD1	2.30	0.65
1:C:78:ARG:NH2	1:C:202:LEU:O	2.29	0.64
1:E:117:TYR:OH	1:E:146:ARG:NH1	2.31	0.63
1:A:205:THR:HG21	1:B:83:ARG:HG3	1.80	0.63
1:E:128:GLN:NE2	1:E:200:GLU:OE2	2.29	0.63
1:A:186:ASP:OD2	1:B:99:GLN:NE2	2.31	0.62
1:C:78:ARG:NH1	1:C:205:THR:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:NH2	1:A:149:GLU:OE1	2.25	0.61
1:A:237:MET:HG2	1:E:50:ILE:HB	1.81	0.61
1:C:194:HIS:HA	1:E:91:ILE:HD13	1.82	0.61
1:D:128:GLN:NE2	1:D:200:GLU:OE2	2.32	0.61
1:D:137:ASP:OD1	1:D:140:ARG:NH2	2.33	0.61
1:E:287:THR:OG1	1:E:289:GLN:OE1	2.14	0.61
1:C:165:GLY:O	1:C:169:GLY:N	2.32	0.61
1:A:236:TYR:HB2	1:E:50:ILE:HG22	1.82	0.61
1:A:96:LEU:HD23	1:A:118:LEU:HD11	1.82	0.61
1:A:211:TYR:OH	1:B:251:SER:O	2.12	0.61
1:B:31:ASN:ND2	1:B:223:CYS:O	2.33	0.61
1:E:101:ARG:NH2	1:E:286:MET:O	2.23	0.60
1:A:28:LEU:O	1:A:32:VAL:HG23	2.01	0.60
1:A:211:TYR:CE2	1:B:255:LEU:HB2	2.36	0.60
1:C:234:LEU:HD22	1:D:52:LEU:HD23	1.83	0.60
1:E:27:ARG:HH21	1:E:220:TYR:HA	1.66	0.60
1:C:25:ILE:HG12	1:C:28:LEU:HD22	1.85	0.59
1:B:232:GLY:O	1:B:235:HIS:NE2	2.35	0.59
1:B:85:LEU:HB3	1:B:195:VAL:HG13	1.83	0.59
1:C:158:ASN:ND2	1:E:286:MET:SD	2.75	0.59
1:A:184:LEU:HD11	1:E:183:GLY:HA2	1.85	0.59
1:B:89:VAL:HG23	1:B:195:VAL:HG11	1.83	0.58
1:A:268:ASN:HD21	1:E:211:TYR:HE2	1.49	0.58
1:B:234:LEU:O	1:B:238:THR:OG1	2.20	0.58
1:C:156:PRO:O	1:C:160:ILE:HG13	2.04	0.58
1:A:23:LYS:O	1:A:27:ARG:NE	2.36	0.58
1:A:42:TYR:HA	1:A:45:TYR:CE1	2.39	0.57
1:A:231:VAL:HA	1:A:238:THR:HG21	1.85	0.57
1:A:234:LEU:HD22	1:E:51:HIS:O	2.03	0.57
1:B:127:HIS:NE2	1:B:137:ASP:OD2	2.37	0.57
1:A:85:LEU:HB3	1:A:195:VAL:HG13	1.87	0.57
1:E:239:PRO:O	1:E:243:VAL:HG12	2.05	0.57
1:B:262:PRO:O	1:B:270:LEU:HB2	2.05	0.57
1:C:43:GLN:HG3	1:C:44:TRP:CD1	2.40	0.57
1:C:201:ARG:NH1	1:E:84:ASN:OD1	2.38	0.57
1:A:126:LYS:NZ	1:A:273:ASN:OD1	2.36	0.57
1:C:155:MET:HG2	1:C:158:ASN:HB3	1.87	0.56
1:D:127:HIS:NE2	1:D:137:ASP:OD2	2.38	0.56
1:E:135:THR:HG22	1:E:151:LEU:CD1	2.34	0.56
1:B:200:GLU:OE2	1:D:94:ARG:NH2	2.28	0.56
1:C:91:ILE:HG12	1:D:197:GLY:HA3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:TYR:HB2	1:D:50:ILE:HG22	1.89	0.55
1:A:89:VAL:HG23	1:A:195:VAL:HG11	1.87	0.55
1:B:49:GLY:O	1:D:235:HIS:HB3	2.06	0.55
1:A:211:TYR:CZ	1:B:255:LEU:HB2	2.42	0.55
1:E:27:ARG:NH2	1:E:224:THR:HG23	2.22	0.55
1:E:213:LEU:HD13	1:E:217:ARG:HD3	1.89	0.54
1:B:153:SER:OG	1:D:285:ASP:OD2	2.23	0.54
1:D:24:ILE:HD12	1:D:250:LEU:O	2.07	0.54
1:A:91:ILE:HD13	1:E:194:HIS:HA	1.89	0.53
1:B:34:MET:HA	1:B:37:ILE:HB	1.90	0.53
1:E:27:ARG:NE	1:E:220:TYR:HD1	2.06	0.53
1:E:79:PHE:CZ	1:E:269:ALA:HB3	2.44	0.53
1:E:90:LEU:HA	1:E:279:ILE:HD13	1.89	0.53
1:A:236:TYR:CD2	1:E:48:LEU:HB2	2.43	0.53
1:C:150:ILE:HD13	1:C:160:ILE:HG12	1.89	0.53
1:A:127:HIS:ND1	1:A:132:THR:OG1	2.38	0.52
1:A:138:LEU:HB3	1:A:147:VAL:HG22	1.90	0.52
1:D:107:GLU:OE2	1:D:176:LYS:NZ	2.32	0.52
1:D:155:MET:SD	1:D:155:MET:N	2.82	0.52
1:E:127:HIS:ND1	1:E:132:THR:OG1	2.33	0.52
1:D:108:HIS:HE1	1:D:287:THR:HB	1.74	0.52
1:A:217:ARG:NH2	1:B:247:TYR:OH	2.43	0.52
1:C:127:HIS:ND1	1:C:132:THR:OG1	2.37	0.52
1:E:216:GLN:NE2	1:E:253:ASP:OD2	2.42	0.52
1:E:28:LEU:HB3	1:E:243:VAL:HG23	1.92	0.51
1:D:271:PRO:HD2	1:D:275:MET:HE3	1.92	0.51
1:E:260:GLU:N	1:E:260:GLU:OE1	2.43	0.51
1:C:28:LEU:HD23	1:C:29:LEU:HD22	1.91	0.51
1:D:127:HIS:ND1	1:D:132:THR:OG1	2.37	0.51
1:E:135:THR:HG22	1:E:151:LEU:HD11	1.91	0.51
1:E:135:THR:O	1:E:139:ARG:HG3	2.09	0.51
1:C:43:GLN:HG3	1:C:44:TRP:HD1	1.75	0.51
1:C:31:ASN:HA	1:C:34:MET:HB2	1.91	0.51
1:A:83:ARG:HE	1:E:201:ARG:HG3	1.77	0.50
1:D:80:VAL:HG13	1:D:83:ARG:HH21	1.74	0.50
1:A:108:HIS:HA	1:A:111:HIS:CG	2.45	0.50
1:E:53:THR:HG22	1:E:54:VAL:H	1.76	0.50
1:A:104:LEU:HD11	1:A:177:LEU:HG	1.92	0.50
1:B:127:HIS:ND1	1:B:132:THR:OG1	2.32	0.50
1:E:53:THR:HG22	1:E:54:VAL:N	2.27	0.50
1:A:133:ASP:OD2	1:A:135:THR:OG1	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ALA:HB1	1:B:263:PHE:CE1	2.46	0.50
1:D:24:ILE:HG23	1:D:25:ILE:HD12	1.93	0.50
1:E:129:LEU:HD11	1:E:199:CYS:HB3	1.94	0.50
1:A:154:SER:HB3	1:B:285:ASP:OD1	2.13	0.49
1:E:189:LEU:HD23	1:E:192:LEU:HD12	1.94	0.49
1:A:113:ARG:NH2	1:A:167:GLU:OE1	2.40	0.49
1:A:135:THR:HG23	1:A:151:LEU:HD11	1.94	0.49
1:A:22:SER:OG	1:A:23:LYS:N	2.41	0.49
1:D:271:PRO:HB2	1:D:274:ALA:HB3	1.94	0.49
1:A:68:LEU:HB3	1:A:252:TRP:HD1	1.77	0.49
1:A:270:LEU:HD22	1:A:275:MET:CE	2.43	0.49
1:D:231:VAL:HG13	1:D:238:THR:HG21	1.95	0.49
1:C:50:ILE:O	1:C:51:HIS:HD2	1.95	0.49
1:D:165:GLY:O	1:D:169:GLY:N	2.35	0.49
1:D:270:LEU:HD22	1:D:275:MET:HE3	1.94	0.49
1:B:103:ILE:HD12	1:B:185:MET:HE3	1.94	0.49
1:C:31:ASN:O	1:C:35:SER:N	2.41	0.49
1:A:183:GLY:HA2	1:A:186:ASP:HB3	1.95	0.49
1:B:41:SER:HB2	1:B:45:TYR:CE2	2.48	0.48
1:A:32:VAL:O	1:A:35:SER:OG	2.25	0.48
1:A:154:SER:OG	1:A:155:MET:N	2.47	0.48
1:C:81:GLU:O	1:C:85:LEU:HG	2.12	0.48
1:B:213:LEU:O	1:B:217:ARG:HD3	2.13	0.48
1:E:37:ILE:HA	1:E:40:ILE:HG12	1.95	0.48
1:C:91:ILE:HD13	1:D:194:HIS:HA	1.95	0.48
1:E:48:LEU:HD23	1:E:48:LEU:H	1.79	0.48
1:E:93:GLU:HB2	1:E:279:ILE:HD11	1.95	0.48
1:A:104:LEU:HD12	1:A:171:LEU:HD13	1.96	0.48
1:C:180:ILE:HD13	1:E:180:ILE:HG13	1.96	0.48
1:A:153:SER:HB2	1:A:159:ARG:HE	1.77	0.48
1:B:52:LEU:HB3	1:B:229:ALA:HA	1.95	0.47
1:B:150:ILE:HD11	1:B:163:LEU:HD12	1.95	0.47
1:E:270:LEU:HA	1:E:270:LEU:HD23	1.50	0.47
1:D:125:LEU:O	1:D:129:LEU:HG	2.15	0.47
1:B:179:ASP:HA	1:B:182:TYR:HB3	1.96	0.47
1:C:262:PRO:O	1:C:270:LEU:HB2	2.14	0.47
1:D:177:LEU:CD1	1:D:182:TYR:HB2	2.41	0.47
1:A:45:TYR:HD2	1:A:50:ILE:HG13	1.78	0.47
1:C:26:PHE:O	1:C:27:ARG:HG2	2.14	0.47
1:A:211:TYR:O	1:A:215:LEU:N	2.47	0.47
1:B:108:HIS:HA	1:B:111:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:O	1:A:220:TYR:HD2	1.97	0.47
1:A:221:LEU:HB3	1:B:244:PHE:CZ	2.50	0.47
1:B:283:LEU:O	1:B:286:MET:HG3	2.15	0.47
1:D:64:ILE:HD11	1:D:218:THR:HG22	1.97	0.47
1:E:81:GLU:HB3	1:E:202:LEU:HD11	1.96	0.47
1:A:180:ILE:HG12	1:E:180:ILE:HD11	1.97	0.47
1:A:236:TYR:HD2	1:E:48:LEU:HB2	1.80	0.47
1:E:27:ARG:HH22	1:E:224:THR:HG23	1.80	0.47
1:E:60:LEU:O	1:E:64:ILE:HG13	2.15	0.47
1:E:79:PHE:HZ	1:E:269:ALA:HB3	1.80	0.47
1:A:42:TYR:HA	1:A:45:TYR:HE1	1.79	0.46
1:A:113:ARG:HE	1:A:167:GLU:CD	2.18	0.46
1:E:31:ASN:ND2	1:E:242:SER:OG	2.48	0.46
1:A:58:SER:HA	1:E:59:LEU:HD13	1.98	0.46
1:B:32:VAL:HG22	1:B:243:VAL:HG11	1.98	0.46
1:C:25:ILE:HG23	1:C:27:ARG:H	1.81	0.46
1:D:189:LEU:O	1:D:193:ALA:N	2.49	0.46
1:C:135:THR:HG22	1:C:139:ARG:HE	1.81	0.46
1:A:180:ILE:HG13	1:B:180:ILE:HG21	1.98	0.46
1:B:214:ILE:HD13	1:D:251:SER:HB3	1.97	0.46
1:D:71:ARG:NH1	1:D:212:THR:HA	2.31	0.46
1:B:239:PRO:O	1:B:243:VAL:HG22	2.16	0.46
1:B:280:GLU:O	1:B:284:LEU:HB2	2.15	0.46
1:E:262:PRO:O	1:E:270:LEU:HD12	2.16	0.46
1:A:190:ASP:OD1	1:B:98:ARG:NH2	2.50	0.46
1:E:274:ALA:O	1:E:278:THR:OG1	2.25	0.46
1:B:86:TRP:CE2	1:B:272:LEU:HD22	2.50	0.45
1:B:190:ASP:OD2	1:D:188:LYS:NZ	2.39	0.45
1:E:206:PRO:HD2	1:E:209:PHE:CE1	2.52	0.45
1:A:91:ILE:HD11	1:E:197:GLY:HA3	1.99	0.45
1:D:188:LYS:HD3	1:D:188:LYS:HA	1.76	0.45
1:C:172:ARG:HE	1:E:103:ILE:HG23	1.82	0.45
1:C:214:ILE:O	1:C:218:THR:OG1	2.25	0.45
1:A:155:MET:SD	1:B:94:ARG:NH2	2.90	0.45
1:A:245:ILE:HG12	1:E:60:LEU:HB2	1.98	0.45
1:B:52:LEU:HD12	1:B:228:PHE:HB3	1.98	0.45
1:C:97:VAL:HG21	1:C:283:LEU:HD22	1.99	0.45
1:A:115:VAL:HG21	1:A:287:THR:HG21	1.98	0.45
1:B:103:ILE:HD13	1:B:181:THR:HB	1.99	0.45
1:B:70:PHE:HE1	1:D:73:SER:HG	1.64	0.45
1:B:74:ALA:HB1	1:D:76:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ASN:OD1	1:C:32:VAL:N	2.49	0.44
1:C:200:GLU:O	1:C:204:THR:OG1	2.33	0.44
1:D:89:VAL:HG23	1:D:195:VAL:HG11	1.98	0.44
1:A:268:ASN:ND2	1:E:211:TYR:HE2	2.15	0.44
1:B:166:ASN:OD1	1:D:102:ASN:ND2	2.50	0.44
1:D:27:ARG:HD3	1:D:27:ARG:HA	1.70	0.44
1:A:129:LEU:HD13	1:A:263:PHE:CD2	2.53	0.44
1:A:180:ILE:HG12	1:E:180:ILE:CD1	2.46	0.44
1:E:280:GLU:O	1:E:284:LEU:HG	2.18	0.44
1:D:52:LEU:HD12	1:D:228:PHE:HB3	1.99	0.44
1:A:201:ARG:HG3	1:B:83:ARG:HD2	2.00	0.44
1:D:262:PRO:O	1:D:270:LEU:HB2	2.18	0.44
1:E:154:SER:HB2	1:E:155:MET:SD	2.58	0.44
1:E:90:LEU:HD12	1:E:279:ILE:HD13	1.99	0.44
1:A:32:VAL:HG22	1:A:243:VAL:HG21	1.99	0.43
1:B:79:PHE:CD1	1:B:262:PRO:HB3	2.53	0.43
1:E:146:ARG:HA	1:E:149:GLU:HG2	2.01	0.43
1:A:244:PHE:CE1	1:E:218:THR:HG23	2.53	0.43
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.74	0.43
1:C:90:LEU:O	1:C:94:ARG:HB2	2.17	0.43
1:C:155:MET:HG2	1:C:158:ASN:CB	2.47	0.43
1:C:90:LEU:HD13	1:C:279:ILE:HG12	2.00	0.43
1:D:37:ILE:HA	1:D:40:ILE:HG12	1.99	0.43
1:D:81:GLU:O	1:D:85:LEU:HG	2.18	0.43
1:B:159:ARG:NH2	1:D:285:ASP:O	2.51	0.43
1:E:269:ALA:O	1:E:271:PRO:HD3	2.18	0.43
1:D:208:PRO:O	1:D:211:TYR:HB2	2.18	0.43
1:E:119:VAL:O	1:E:123:TRP:HD1	2.01	0.43
1:B:156:PRO:O	1:B:160:ILE:HG13	2.19	0.42
1:A:234:LEU:HD21	1:E:53:THR:H	1.84	0.42
1:A:236:TYR:O	1:A:239:PRO:HD2	2.19	0.42
1:D:42:TYR:CE1	1:D:45:TYR:CE2	3.07	0.42
1:D:214:ILE:O	1:D:218:THR:OG1	2.19	0.42
1:A:180:ILE:HG21	1:E:180:ILE:HD13	2.00	0.42
1:B:41:SER:O	1:B:44:TRP:N	2.52	0.42
1:D:28:LEU:HG	1:D:250:LEU:HD12	2.00	0.42
1:E:71:ARG:NH2	1:E:253:ASP:OD1	2.48	0.42
1:E:164:ALA:O	1:E:168:ILE:HG12	2.19	0.42
1:E:223:CYS:SG	1:E:246:SER:HA	2.59	0.42
1:E:265:THR:O	1:E:268:ASN:ND2	2.51	0.42
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.88	0.42
1:B:254:SER:O	1:B:257:GLU:HG2	2.19	0.42
1:C:190:ASP:OD1	1:C:191:GLU:N	2.53	0.42
1:C:35:SER:HA	1:C:227:PRO:HB2	2.01	0.42
1:A:50:ILE:HB	1:B:237:MET:HG2	2.02	0.42
1:C:284:LEU:HA	1:C:287:THR:HG23	2.01	0.42
1:E:57:PHE:O	1:E:61:GLY:N	2.41	0.42
1:A:89:VAL:CG2	1:A:195:VAL:HG11	2.50	0.42
1:B:180:ILE:HD12	1:B:180:ILE:H	1.84	0.42
1:C:234:LEU:HD11	1:D:56:PRO:HG2	2.02	0.42
1:C:244:PHE:CE1	1:D:221:LEU:HD23	2.55	0.42
1:C:119:VAL:HG22	1:C:283:LEU:HD12	2.02	0.42
1:C:282:ASN:O	1:C:286:MET:HG3	2.20	0.42
1:E:83:ARG:CD	1:E:270:LEU:HD21	2.50	0.42
1:D:260:GLU:C	1:D:262:PRO:HD3	2.40	0.42
1:A:81:GLU:O	1:A:85:LEU:HG	2.20	0.41
1:D:24:ILE:HG13	1:D:250:LEU:HB3	2.01	0.41
1:E:93:GLU:HB3	1:E:283:LEU:HD11	2.01	0.41
1:C:172:ARG:NH2	1:C:179:ASP:OD1	2.53	0.41
1:C:230:LEU:HD22	1:D:56:PRO:HG3	2.02	0.41
1:C:252:TRP:CH2	1:D:215:LEU:HD21	2.56	0.41
1:E:135:THR:HG22	1:E:151:LEU:HD13	2.01	0.41
1:A:82:ALA:HB1	1:A:263:PHE:CE1	2.55	0.41
1:E:171:LEU:HD22	1:E:176:LYS:HD2	2.02	0.41
1:E:213:LEU:O	1:E:217:ARG:HB2	2.20	0.41
1:A:36:ILE:O	1:A:40:ILE:HG23	2.21	0.41
1:A:183:GLY:HA3	1:B:184:LEU:HD21	2.02	0.41
1:C:36:ILE:O	1:C:40:ILE:HG23	2.20	0.41
1:C:223:CYS:SG	1:C:246:SER:OG	2.79	0.41
1:D:172:ARG:NH2	1:D:179:ASP:OD2	2.53	0.41
1:A:180:ILE:H	1:A:180:ILE:HD12	1.85	0.41
1:D:150:ILE:HD13	1:D:160:ILE:HG12	2.03	0.41
1:E:35:SER:OG	1:E:239:PRO:HB3	2.20	0.41
1:C:137:ASP:OD1	1:C:140:ARG:NH2	2.46	0.41
1:E:83:ARG:HD3	1:E:270:LEU:HD21	2.03	0.41
1:A:272:LEU:HD23	1:A:275:MET:SD	2.61	0.41
1:B:97:VAL:HG21	1:B:283:LEU:HG	2.03	0.41
1:A:200:GLU:OE2	1:B:94:ARG:NH2	2.46	0.41
1:B:28:LEU:HG	1:B:247:TYR:HD1	1.85	0.41
1:C:126:LYS:HD3	1:C:130:ARG:HG3	2.02	0.41
1:C:172:ARG:HA	1:C:177:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:GLN:HB2	1:E:48:LEU:H	1.73	0.41
1:A:98:ARG:HG3	1:E:162:LEU:HD12	2.02	0.41
1:C:59:LEU:HD13	1:E:58:SER:HA	2.02	0.41
1:C:234:LEU:O	1:C:237:MET:N	2.54	0.41
1:D:42:TYR:CZ	1:D:45:TYR:CE2	3.09	0.41
1:E:52:LEU:HD23	1:E:52:LEU:HA	1.85	0.41
1:E:238:THR:N	1:E:239:PRO:HD2	2.36	0.41
1:A:60:LEU:HD21	1:B:244:PHE:CD2	2.56	0.40
1:A:214:ILE:O	1:A:218:THR:OG1	2.27	0.40
1:B:126:LYS:HG3	1:B:127:HIS:N	2.36	0.40
1:D:95:THR:HB	1:D:98:ARG:HH21	1.86	0.40
1:A:134:PRO:O	1:A:138:LEU:HD13	2.20	0.40
1:B:125:LEU:O	1:B:129:LEU:HG	2.20	0.40
1:C:42:TYR:O	1:C:45:TYR:HD2	2.03	0.40
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.51	0.40
1:B:207:VAL:HG22	1:B:260:GLU:OE2	2.21	0.40
1:D:95:THR:HA	1:D:98:ARG:HB3	2.03	0.40
1:D:115:VAL:O	1:D:119:VAL:HG23	2.21	0.40
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.48	0.40
1:D:237:MET:SD	1:D:240:PHE:HD1	2.45	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	266/296 (90%)	256 (96%)	8 (3%)	2 (1%)	19	56
1	B	264/296 (89%)	251 (95%)	13 (5%)	0	100	100
1	C	263/296 (89%)	250 (95%)	7 (3%)	6 (2%)	6	37
1	D	266/296 (90%)	254 (96%)	9 (3%)	3 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	268/296 (90%)	252 (94%)	12 (4%)	4 (2%)	10	44
All	All	1327/1480 (90%)	1263 (95%)	49 (4%)	15 (1%)	14	50

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	HIS
1	D	266	ALA
1	E	235	HIS
1	E	271	PRO
1	C	28	LEU
1	C	42	TYR
1	C	173	GLU
1	E	47	GLN
1	E	49	GLY
1	A	235	HIS
1	C	174	ALA
1	D	210	ALA
1	A	48	LEU
1	C	206	PRO
1	D	288	GLY

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	228/258 (88%)	220 (96%)	8 (4%)	36	63
1	B	226/258 (88%)	216 (96%)	10 (4%)	28	57
1	C	222/258 (86%)	218 (98%)	4 (2%)	59	77
1	D	227/258 (88%)	222 (98%)	5 (2%)	52	72
1	E	234/258 (91%)	227 (97%)	7 (3%)	41	65
All	All	1137/1290 (88%)	1103 (97%)	34 (3%)	41	65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	79	PHE
1	A	126	LYS
1	A	131	LYS
1	A	159	ARG
1	A	213	LEU
1	A	220	TYR
1	A	244	PHE
1	B	26	PHE
1	B	34	MET
1	B	44	TRP
1	B	45	TYR
1	B	48	LEU
1	B	83	ARG
1	B	108	HIS
1	B	126	LYS
1	B	236	TYR
1	B	286	MET
1	C	28	LEU
1	C	112	ARG
1	C	126	LYS
1	C	223	CYS
1	D	45	TYR
1	D	126	LYS
1	D	155	MET
1	D	211	TYR
1	D	259	LEU
1	E	46	GLU
1	E	109	ASP
1	E	155	MET
1	E	209	PHE
1	E	211	TYR
1	E	273	ASN
1	E	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	31	ASN
1	C	51	HIS
1	D	72	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 9 ligands modelled in this entry, 9 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(Å²)	Q<0.9
1	A	268/296 (90%)	-0.15	11 (4%)	37	31	82, 114, 155, 182	0
1	B	266/296 (89%)	-0.12	4 (1%)	73	68	74, 105, 153, 172	0
1	C	265/296 (89%)	-0.08	9 (3%)	45	37	73, 107, 150, 175	0
1	D	268/296 (90%)	-0.23	1 (0%)	92	91	78, 105, 147, 186	0
1	E	270/296 (91%)	-0.30	7 (2%)	56	47	81, 116, 164, 193	0
All	All	1337/1480 (90%)	-0.18	32 (2%)	59	51	73, 110, 155, 193	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	GLN	5.1
1	C	53	THR	4.6
1	C	48	LEU	4.4
1	A	52	LEU	4.0
1	C	49	GLY	3.9
1	E	49	GLY	3.5
1	C	50	ILE	3.4
1	A	51	HIS	3.4
1	A	24	ILE	3.3
1	A	289	GLN	3.2
1	E	290	HIS	3.1
1	B	236	TYR	3.0
1	E	291	PRO	2.8
1	B	265	THR	2.7
1	A	53	THR	2.6
1	C	217	ARG	2.5
1	D	174	ALA	2.5
1	E	47	GLN	2.5
1	E	292	LEU	2.5
1	B	267	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	26	PHE	2.5
1	A	212	THR	2.4
1	C	98	ARG	2.4
1	C	51	HIS	2.4
1	A	262	PRO	2.3
1	A	44	TRP	2.3
1	E	293	PRO	2.3
1	E	211	TYR	2.3
1	B	95	THR	2.1
1	A	216	GLN	2.1
1	C	106	ALA	2.1
1	A	45	TYR	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
2	ZN	C	301	1/1	0.92	0.05	104,104,104,104	0
2	ZN	A	301	1/1	0.94	0.17	119,119,119,119	0
2	ZN	B	301	1/1	0.95	0.05	108,108,108,108	0
2	ZN	D	301	1/1	0.95	0.06	101,101,101,101	0
2	ZN	A	303	1/1	0.96	0.11	134,134,134,134	0
2	ZN	E	301	1/1	0.96	0.13	104,104,104,104	0
2	ZN	E	302	1/1	0.96	0.06	150,150,150,150	0
2	ZN	D	302	1/1	0.97	0.11	123,123,123,123	0
2	ZN	A	302	1/1	0.98	0.10	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.