



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:24 pm BST

PDB ID : 3BDK  
Title : Crystal Structure of Streptococcus suis mannonate dehydratase complexed with substrate analogue  
Authors : Gao, F.; Zhang, Q.M.; Peng, H.; Liu, Y.W.; Qi, J.X.; Gao, G.F.  
Deposited on : 2007-11-15  
Resolution : 2.50 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

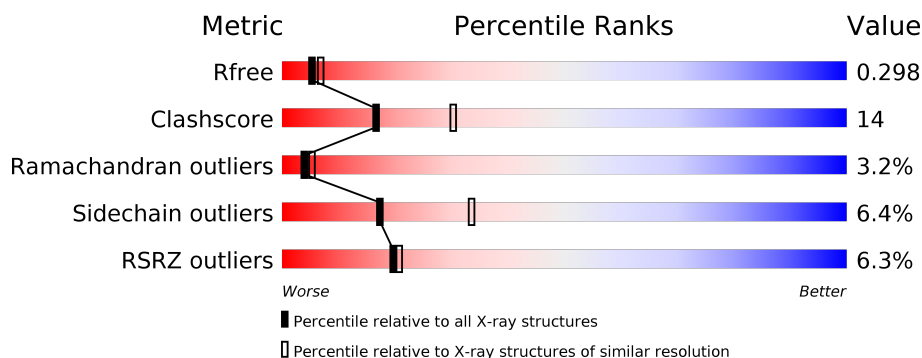
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	386	
1	B	386	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5525 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 D-mannonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2738	1745	465	514	14			
1	B	349	Total	C	N	O	S	0	0	0
			2733	1742	465	513	13			

There are 40 discrepancies between the modelled and reference sequences:

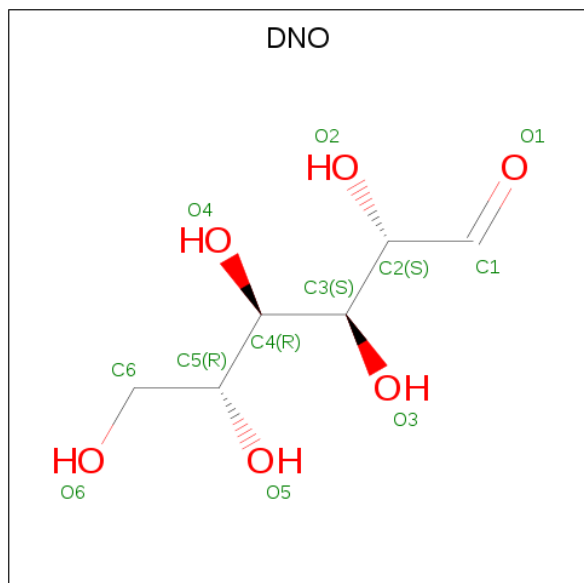
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A4VVI4
A	2	GLY	-	EXPRESSION TAG	UNP A4VVI4
A	3	SER	-	EXPRESSION TAG	UNP A4VVI4
A	4	SER	-	EXPRESSION TAG	UNP A4VVI4
A	5	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	6	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	7	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	8	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	9	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	10	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	11	SER	-	EXPRESSION TAG	UNP A4VVI4
A	12	SER	-	EXPRESSION TAG	UNP A4VVI4
A	13	GLY	-	EXPRESSION TAG	UNP A4VVI4
A	14	LEU	-	EXPRESSION TAG	UNP A4VVI4
A	15	VAL	-	EXPRESSION TAG	UNP A4VVI4
A	16	PRO	-	EXPRESSION TAG	UNP A4VVI4
A	17	ARG	-	EXPRESSION TAG	UNP A4VVI4
A	18	GLY	-	EXPRESSION TAG	UNP A4VVI4
A	19	SER	-	EXPRESSION TAG	UNP A4VVI4
A	20	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	1	MET	-	EXPRESSION TAG	UNP A4VVI4
B	2	GLY	-	EXPRESSION TAG	UNP A4VVI4
B	3	SER	-	EXPRESSION TAG	UNP A4VVI4
B	4	SER	-	EXPRESSION TAG	UNP A4VVI4
B	5	HIS	-	EXPRESSION TAG	UNP A4VVI4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	7	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	8	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	9	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	10	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	11	SER	-	EXPRESSION TAG	UNP A4VVI4
B	12	SER	-	EXPRESSION TAG	UNP A4VVI4
B	13	GLY	-	EXPRESSION TAG	UNP A4VVI4
B	14	LEU	-	EXPRESSION TAG	UNP A4VVI4
B	15	VAL	-	EXPRESSION TAG	UNP A4VVI4
B	16	PRO	-	EXPRESSION TAG	UNP A4VVI4
B	17	ARG	-	EXPRESSION TAG	UNP A4VVI4
B	18	GLY	-	EXPRESSION TAG	UNP A4VVI4
B	19	SER	-	EXPRESSION TAG	UNP A4VVI4
B	20	HIS	-	EXPRESSION TAG	UNP A4VVI4

- Molecule 2 is D-mannose (three-letter code: DNO) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	19	Total 19	O 19	0	0

These plots are drawn for all protein, RNA and DNA 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.

Chain A:

62% 23% 5% 10%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY VAL PRO ARG GLY S19 S24 F25 R26 T35 L36 Q46 Q47 I48 V49 D54 V55 P56 P57 G58 Q59 A60 A61 P62 L63 E64 N65 I66 L67 E68 K71 L78 E79 I80 T81 V82 I83 E84 S85 I86 N98 A101 I102 E104 K107 S109 T110 R111 A115 A116 G117 I118 P119 V120 V121 C122 Y123 M124 W131 S134 S144 L154 V157 D158 P159 VAL ALA ASP ASP LEU ASN LEU LEU PRO GLY TRP ASP SER SER TYR S174 A180 W195 E199 K203 T206 P207 E211 A217 I218 H219 P220 D221 D222 P223 P224 T234 E238 R242 F243 L244 N245 L246 Y247 D248 S249 E250 C257 Y261 D264 P265 K266 N267 M272 T273 E274 Y275 R279 N280 K281 I282 N283 F284 N285 H286 T287 R288 N289 E299 I309 D310 N311 N312 A313 V314 V315 L318 V319 S326 L327 R328 P329 D330 H331 G332 G333 R334 I335 W336 P343 G344 Y345 D349 R350 A351 L352 L360 N364 M365 K370 F374 G375 L376 K377 A378 V381 GLY THR LYS GLU GLY

Chain B:

8% 66% 22% 10%

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.47Å 105.47Å 160.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.27 – 2.50 45.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (45.27-2.50) 95.3 (45.25-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.250 , 0.303 0.249 , 0.298	Depositor DCC
$R_{free}$ test set	1550 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DNO, MN

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	0.61	1/2805 (0.0%)	0.65	0/3808
1	B	0.56	0/2800	0.71	0/3802
All	All	0.59	1/5605 (0.0%)	0.68	0/7610

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	ILE	CG1-CD1	14.03	2.47	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	SER	Peptide
1	B	84	GLU	Peptide



## 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	2738	0	2676	98	0
1	B	2733	0	2679	61	0
2	A	12	0	11	1	0
3	A	1	0	0	0	0
4	A	22	0	0	1	0
4	B	19	0	0	0	0
All	All	5525	0	5366	154	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 (154) 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:250:GLU:HG2	1:A:280:ASN:HD22	1.25	1.00
1:A:319:VAL:HG13	1:A:365:MET:HE3	1.46	0.97
1:A:286:HIS:ND1	1:A:330:ASP:OD2	1.99	0.95
1:A:218:ILE:CG1	1:A:218:ILE:CD1	2.47	0.93
1:A:250:GLU:HG3	1:A:281:ARG:NH1	1.91	0.85
1:A:287:THR:O	1:A:287:THR:HG23	1.76	0.83
1:A:63:LEU:HD22	1:A:67:LEU:HG	1.60	0.83
1:A:199:GLU:HG2	1:A:203:LYS:NZ	1.93	0.83
1:A:319:VAL:HG13	1:A:365:MET:CE	2.10	0.81
1:B:312:ASN:ND2	1:B:364:ASN:HD21	1.79	0.80
1:B:131:TRP:HA	1:B:222:ASP:O	1.84	0.78
1:A:199:GLU:HG3	1:A:246:LEU:HD22	1.66	0.77
1:B:287:THR:HG23	1:B:287:THR:O	1.83	0.77
1:A:315:VAL:HG11	1:A:360:LEU:HB3	1.69	0.74
1:B:284:PHE:CE1	1:B:286:HIS:HE1	2.04	0.74
1:B:137:HIS:HD2	1:B:334:ARG:HH21	1.37	0.72
1:B:59:GLN:O	1:B:60:ALA:HB3	1.90	0.72
1:A:36:LEU:H	1:A:36:LEU:HD12	1.56	0.70
1:A:66:ILE:HD11	1:A:116:ALA:CB	2.22	0.70
1:A:319:VAL:CG1	1:A:365:MET:HE3	2.20	0.70
1:B:214:VAL:O	1:B:251:HIS:HD2	1.75	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLU:HG2	1:A:203:LYS:HZ3	1.55	0.69
1:B:312:ASN:HD21	1:B:364:ASN:HD21	1.42	0.67
1:B:182:ILE:HG22	1:B:186:ARG:HD2	1.77	0.67
1:B:202:ILE:HD11	1:B:246:LEU:HB3	1.77	0.65
1:B:274:GLU:HG3	1:B:317:LEU:HD22	1.81	0.63
1:A:311:MET:O	1:A:315:VAL:HG12	1.97	0.63
1:A:328:ARG:NH2	1:A:345:TYR:OH	2.32	0.63
1:B:219:HIS:HD2	1:B:220:PRO:O	1.82	0.63
1:B:383:THR:O	1:B:384:LYS:HB2	1.99	0.62
1:A:312:ASN:ND2	1:A:364:ASN:HD21	1.98	0.61
1:A:57:VAL:HG13	1:A:58:GLY:N	2.15	0.61
1:A:101:ALA:O	1:A:104:GLU:HB2	2.01	0.61
1:A:221:ASP:HB2	1:A:234:ILE:O	2.01	0.61
1:B:287:THR:HG21	1:B:327:LEU:HD21	1.83	0.60
1:A:211:GLU:HB2	4:A:405:HOH:O	2.02	0.59
1:A:376:ILE:HD13	1:B:305:GLN:HB3	1.85	0.58
1:B:331:HIS:HA	1:B:344:GLY:O	2.03	0.58
1:A:66:ILE:HD11	1:A:116:ALA:HB2	1.86	0.58
1:A:352:LEU:HD23	1:B:352:LEU:HD23	1.86	0.58
1:A:26:ARG:NH1	1:A:84:GLU:HG2	2.18	0.57
1:B:59:GLN:O	1:B:60:ALA:CB	2.51	0.57
1:A:199:GLU:HG2	1:A:203:LYS:HZ1	1.65	0.57
1:B:263:SER:HB3	1:B:297:PHE:CD1	2.40	0.57
1:B:257:CYS:HA	1:B:286:HIS:HB2	1.87	0.56
1:B:85:SER:HA	1:B:122:CYS:O	2.05	0.56
1:B:353:GLY:O	1:B:357:PHE:HD2	1.88	0.56
1:B:126:MET:HG3	1:B:221:ASP:OD2	2.06	0.55
1:A:250:GLU:HG3	1:A:281:ARG:CZ	2.36	0.55
1:A:122:CYS:HA	1:A:217:ALA:O	2.07	0.55
1:A:279:ARG:O	1:A:281:ARG:NH1	2.39	0.55
1:A:286:HIS:CE1	1:A:328:ARG:NH1	2.75	0.55
1:A:57:VAL:HG13	1:A:58:GLY:H	1.72	0.55
1:B:137:HIS:CD2	1:B:334:ARG:HH21	2.23	0.54
1:A:56:PRO:O	1:A:57:VAL:HB	2.06	0.54
1:B:287:THR:CG2	1:B:287:THR:O	2.54	0.54
1:A:333:ARG:HD3	1:A:349:ASP:OD2	2.07	0.54
1:B:287:THR:HG23	1:B:357:PHE:CZ	2.43	0.54
1:A:365:MET:CE	1:A:365:MET:HA	2.38	0.54
1:B:153:ASP:O	1:B:155:ALA:N	2.38	0.53
1:B:265:PRO:O	1:B:267:ASN:N	2.42	0.53
1:B:286:HIS:CD2	1:B:330:ASP:OD2	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:CD1	2:A:387:DNO:H1	2.45	0.52
1:A:250:GLU:HG2	1:A:280:ASN:ND2	2.09	0.51
1:A:283:ASN:O	1:A:284:PHE:HB2	2.10	0.51
1:A:248:ASP:OD1	1:A:279:ARG:NH1	2.44	0.50
1:A:83:ILE:HG13	1:A:118:ILE:HG21	1.92	0.50
1:A:287:THR:O	1:A:287:THR:CG2	2.49	0.50
1:A:144:SER:HB2	1:A:335:ILE:HG22	1.93	0.50
1:A:24:SER:OG	1:A:326:SER:HB2	2.11	0.50
1:A:131:TRP:HA	1:A:222:ASP:O	2.12	0.49
1:A:82:VAL:HG22	1:A:120:VAL:HB	1.94	0.49
1:B:244:LEU:HD23	1:B:279:ARG:HD3	1.94	0.49
1:B:314:VAL:O	1:B:317:LEU:HB2	2.13	0.49
1:B:224:PRO:HD3	1:B:263:SER:HB2	1.93	0.49
1:B:57:VAL:HG13	1:B:87:PRO:HB2	1.95	0.49
1:B:353:GLY:O	1:B:357:PHE:CD2	2.66	0.48
1:A:195:TRP:CZ3	1:A:242:ARG:HD2	2.49	0.48
1:B:127:PRO:HB3	1:B:185:TYR:CZ	2.49	0.48
1:A:220:PRO:HB3	1:A:261:TYR:CZ	2.49	0.47
1:A:264:ASP:OD1	1:A:266:LYS:HG2	2.14	0.47
1:B:284:PHE:CE1	1:B:286:HIS:CE1	2.93	0.47
1:A:86:ILE:HD13	1:A:109:SER:HB3	1.95	0.47
1:A:312:ASN:HD22	1:A:360:LEU:HD22	1.79	0.47
1:A:26:ARG:CZ	1:A:84:GLU:HG2	2.45	0.47
1:A:352:LEU:HB3	1:B:355:THR:HG21	1.97	0.47
1:B:137:HIS:HD2	1:B:334:ARG:NH2	2.08	0.47
1:B:224:PRO:HG2	1:B:264:ASP:HB2	1.97	0.46
1:A:104:GLU:OE2	1:A:107:LYS:NZ	2.48	0.46
1:A:365:MET:HE2	1:A:370:LYS:HB2	1.97	0.46
1:A:85:SER:HA	1:A:122:CYS:O	2.15	0.46
1:A:244:LEU:HG	1:A:281:ARG:HG3	1.96	0.46
1:B:288:ARG:HB3	1:B:330:ASP:O	2.15	0.46
1:B:91:ASP:HB2	1:B:102:LEU:CD1	2.46	0.46
1:A:207:PRO:O	1:A:211:GLU:HB3	2.16	0.46
1:A:299:GLU:OE1	1:A:331:HIS:HB2	2.16	0.46
1:B:220:PRO:HB3	1:B:261:TYR:CZ	2.50	0.46
1:A:57:VAL:CG1	1:A:58:GLY:N	2.79	0.45
1:A:25:PHE:CZ	1:A:350:ARG:HB3	2.50	0.45
1:A:46:GLN:O	1:A:78:LEU:HD22	2.15	0.45
1:B:289:ASN:OD1	1:B:309:ILE:HB	2.17	0.45
1:A:26:ARG:HA	1:A:49:VAL:O	2.17	0.45
1:A:285:MET:HB2	1:A:327:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:C	1:A:327:LEU:HD23	2.36	0.45
1:A:352:LEU:HD21	1:B:351:ALA:HB1	1.97	0.45
1:A:218:ILE:O	1:A:218:ILE:HG23	2.16	0.45
1:A:376:ILE:HG21	1:B:305:GLN:HG2	1.98	0.45
1:A:24:SER:HA	1:A:47:GLY:O	2.17	0.44
1:A:288:ARG:HB2	1:A:330:ASP:HB3	1.99	0.44
1:A:57:VAL:CG1	1:A:58:GLY:H	2.29	0.44
1:A:328:ARG:HA	1:A:329:PRO:HD2	1.75	0.44
1:A:312:ASN:HD21	1:A:364:ASN:HD21	1.66	0.44
1:B:126:MET:HB3	1:B:129:PHE:O	2.17	0.44
1:B:265:PRO:C	1:B:267:ASN:N	2.70	0.43
1:B:66:ILE:HG12	1:B:66:ILE:H	1.66	0.43
1:A:80:ILE:HB	1:A:118:ILE:HG12	2.00	0.43
1:A:257:CYS:HA	1:A:286:HIS:HB2	2.00	0.43
1:A:365:MET:HA	1:A:365:MET:HE3	2.01	0.43
1:B:32:ASP:OD1	1:B:34:VAL:HG13	2.19	0.43
1:A:49:VAL:CG1	1:A:84:GLU:HB2	2.49	0.43
1:A:286:HIS:NE2	1:A:328:ARG:NH1	2.66	0.43
1:A:285:MET:HE3	1:A:318:LEU:HD11	2.01	0.43
1:A:330:ASP:O	1:A:331:HIS:C	2.58	0.43
1:B:60:ALA:HB2	1:B:105:ASN:HB3	1.99	0.42
1:B:355:THR:HA	1:B:358:ASN:ND2	2.33	0.42
1:A:103:ILE:O	1:A:107:LYS:HG2	2.19	0.42
1:B:361:TYR:O	1:B:365:MET:HG2	2.18	0.42
1:A:104:GLU:O	1:A:107:LYS:HB2	2.19	0.42
1:B:241:GLU:HG3	1:B:275:TYR:OH	2.20	0.42
1:B:227:ILE:HD12	1:B:228:PHE:CD2	2.54	0.42
1:A:124:ASN:OD1	1:A:124:ASN:C	2.58	0.42
1:A:199:GLU:O	1:A:203:LYS:HG2	2.19	0.42
1:A:285:MET:HE2	1:A:318:LEU:HD21	2.02	0.42
1:A:108:THR:HG23	1:A:111:ARG:HH11	1.84	0.42
1:A:289:ASN:HA	1:A:309:ILE:HD12	2.01	0.42
1:A:274:GLU:O	1:A:275:TYR:C	2.59	0.41
1:A:334:ARG:HG3	1:A:334:ARG:HH11	1.84	0.41
1:B:86:ILE:HD13	1:B:109:SER:HB3	2.00	0.41
1:B:49:VAL:HG22	1:B:82:VAL:HB	2.02	0.41
1:A:257:CYS:HB2	1:A:286:HIS:HB2	2.02	0.41
1:A:24:SER:HG	1:A:326:SER:HB2	1.84	0.41
1:B:137:HIS:CD2	1:B:334:ARG:NH2	2.87	0.41
1:A:267:ASN:HB3	1:A:272:MET:HE1	2.02	0.41
1:A:335:ILE:HG12	1:A:336:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HB3	1:A:247:TYR:CE1	2.56	0.41
1:B:96:LYS:HA	1:B:97:PRO:HD2	1.75	0.41
1:A:54:ASP:OD1	1:A:54:ASP:N	2.53	0.41
1:A:122:CYS:SG	1:A:219:HIS:HB2	2.61	0.41
1:A:374:PHE:C	1:A:376:ILE:H	2.25	0.40
1:B:289:ASN:HA	1:B:309:ILE:HD12	2.01	0.40
1:A:374:PHE:HB2	1:A:376:ILE:HD12	2.04	0.40
1:B:340:THR:HB	1:B:346:GLY:HA2	2.03	0.40
1:B:94:GLN:OE1	1:B:184:ASN:ND2	2.48	0.40
1:A:257:CYS:CB	1:A:286:HIS:HB2	2.51	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	345/386 (89%)	298 (86%)	37 (11%)	10 (3%)	4	6
1	B	345/386 (89%)	306 (89%)	27 (8%)	12 (4%)	3	4
All	All	690/772 (89%)	604 (88%)	64 (9%)	22 (3%)	4	5

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	343	PRO
1	B	85	SER
1	B	128	VAL
1	B	154	LEU
1	B	330	ASP
1	B	343	PRO
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	247	TYR
1	B	60	ALA
1	B	266	LYS
1	B	331	HIS
1	B	341	LYS
1	A	85	SER
1	B	155	ALA
1	B	384	LYS
1	B	338	ASP
1	A	248	ASP
1	A	330	ASP
1	A	331	HIS
1	A	314	VAL
1	A	224	PRO

### 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	288/321 (90%)	266 (92%)	22 (8%)	13	25
1	B	288/321 (90%)	273 (95%)	15 (5%)	23	44
All	All	576/642 (90%)	539 (94%)	37 (6%)	17	33

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	36	LEU
1	A	55	VAL
1	A	63	LEU
1	A	64	GLU
1	A	66	ILE
1	A	68	GLU
1	A	80	ILE
1	A	85	SER

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Mol	Chain	Res	Type
1	A	107	LYS
1	A	134	SER
1	A	154	LEU
1	A	206	LEU
1	A	211	GLU
1	A	238	GLU
1	A	242	ARG
1	A	244	LEU
1	A	250	GLU
1	A	330	ASP
1	A	335	ILE
1	A	350	ARG
1	A	365	MET
1	B	34	VAL
1	B	128	VAL
1	B	206	LEU
1	B	227	ILE
1	B	242	ARG
1	B	244	LEU
1	B	269	VAL
1	B	280	ASN
1	B	286	HIS
1	B	287	THR
1	B	303	LEU
1	B	315	VAL
1	B	328	ARG
1	B	331	HIS
1	B	371	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	280	ASN
1	A	283	ASN
1	A	298	GLN
1	A	312	ASN
1	A	324	GLN
1	B	105	ASN
1	B	137	HIS
1	B	138	HIS
1	B	219	HIS

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Mol	Chain	Res	Type
1	B	251	HIS
1	B	283	ASN
1	B	286	HIS
1	B	298	GLN
1	B	312	ASN
1	B	324	GLN
1	B	331	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
2	DNO	A	387	3	10,11,11	1.08	1 (10%)	13,14,14	2.01	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DNO	A	387	3	-	8/14/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	387	DNO	C3-C2	2.10	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	387	DNO	C4-C3-C2	4.58	121.53	113.54
2	A	387	DNO	C5-C4-C3	4.52	119.54	112.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	387	DNO	O3-C3-C4-O4
2	A	387	DNO	C4-C5-C6-O6
2	A	387	DNO	O5-C5-C6-O6
2	A	387	DNO	C2-C3-C4-C5
2	A	387	DNO	C3-C4-C5-C6
2	A	387	DNO	C2-C3-C4-O4
2	A	387	DNO	C3-C4-C5-O5
2	A	387	DNO	O3-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	387	DNO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	349/386 (90%)	0.35	13 (3%) 41 45	23, 46, 70, 76	0
1	B	349/386 (90%)	0.30	31 (8%) 9 9	22, 41, 65, 95	0
All	All	698/772 (90%)	0.32	44 (6%) 20 21	22, 42, 69, 95	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	GLY	6.0
1	B	293	GLY	5.9
1	B	148	ALA	5.3
1	B	154	LEU	4.3
1	B	383	THR	4.2
1	A	115	ALA	3.8
1	B	339	GLN	3.7
1	A	64	GLU	3.7
1	B	132	THR	3.6
1	A	61	TRP	3.6
1	B	149	PHE	3.5
1	B	152	SER	3.5
1	B	155	ALA	3.4
1	B	159	PRO	3.1
1	B	186	ARG	3.0
1	A	180	ALA	2.8
1	A	286	HIS	2.8
1	B	133	ARG	2.7
1	B	147	LEU	2.7
1	B	157	VAL	2.7
1	A	378	ALA	2.7
1	B	225	TYR	2.7
1	B	150	LEU	2.6
1	A	111	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	71	LYS	2.6
1	B	158	ASP	2.6
1	B	297	PHE	2.5
1	B	384	LYS	2.5
1	B	292	ALA	2.4
1	B	134	SER	2.4
1	B	228	PHE	2.4
1	B	183	GLU	2.3
1	B	344	GLY	2.3
1	B	31	LYS	2.3
1	A	219	HIS	2.3
1	B	30	LYS	2.2
1	A	157	VAL	2.2
1	A	60	ALA	2.1
1	B	290	VAL	2.1
1	A	343	PRO	2.1
1	B	295	TRP	2.1
1	B	187	GLN	2.0
1	B	340	THR	2.0
1	A	118	ILE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MN	A	388	1/1	0.48	0.35	100,100,100,100	0
2	DNO	A	387	12/12	0.85	0.21	74,76,77,77	0

## 6.5 Other polymers

There are no such residues in this entry.