



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:35 AM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

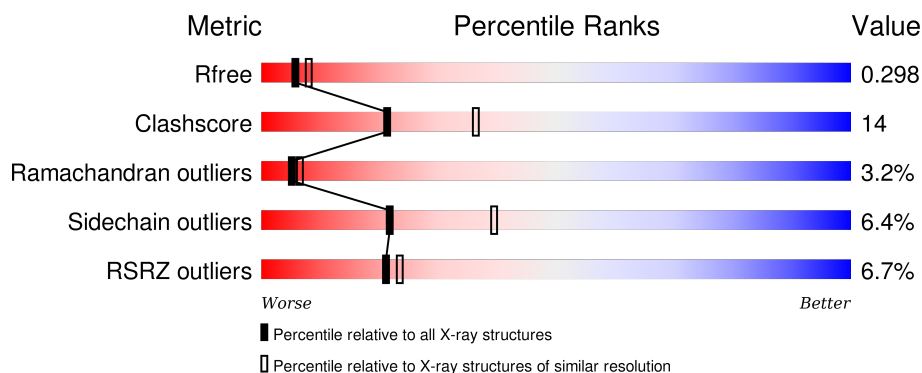
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>62%</div> <div>23%</div> <div>5%</div> <div>10%</div> </div>
1	B	386	<div> <div>8%</div> <div>66%</div> <div>22%</div> <div>•</div> <div>10%</div> </div>

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
3	MN	A	388	-	-	-	X

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:

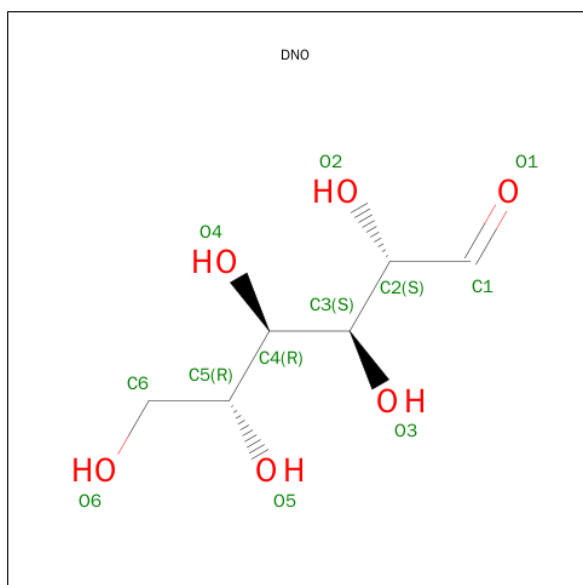
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A4VVI4
A	2	GLY	-	EXPRESSION TAG	UNP A4VVI4
A	3	SER	-	EXPRESSION TAG	UNP A4VVI4
A	4	SER	-	EXPRESSION TAG	UNP A4VVI4
A	5	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	6	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	7	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	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 SUGAR (D-MANNOSE) (three-letter code: DNO) (formula: C₆H₁₂O₆).



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.38%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 30371 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5525	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:59:GLN:O	1:B:60:ALA:HB3	1.90	0.72
1:B:137:HIS:HD2	1:B:334:ARG:HH21	1.37	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:B:331:HIS:HA	1:B:344:GLY:O	2.03	0.58
1:A:376:ILE:HD13	1:B:305:GLN:HB3	1.85	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:B:287:THR:CG2	1:B:287:THR:O	2.54	0.54
1:A:56:PRO:O	1:A:57:VAL:HB	2.06	0.54
1:B:287:THR:HG23	1:B:357:PHE:CZ	2.43	0.54
1:A:333:ARG:HD3	1:A:349:ASP:OD2	2.07	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:B:284:PHE:CE1	1:B:286:HIS:CE1	2.93	0.47
1:A:264:ASP:OD1	1:A:266:LYS:HG2	2.14	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:365:MET:HE2	1:A:370:LYS:HB2	1.97	0.46
1:A:104:GLU:OE2	1:A:107:LYS:NZ	2.48	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: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:207:PRO:O	1:A:211:GLU:HB3	2.16	0.46
1:A:57:VAL:CG1	1:A:58:GLY:N	2.79	0.45
1:A:46:GLN:O	1:A:78:LEU:HD22	2.15	0.45
1:A:25:PHE:CZ	1:A:350:ARG:HB3	2.50	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:352:LEU:HD21	1:B:351:ALA:HB1	1.97	0.45
1:A:327:LEU:C	1:A:327:LEU:HD23	2.36	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: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:24:SER:HA	1:A:47:GLY:O	2.17	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:365:MET:HA	1:A:365:MET:HE3	2.01	0.43
1:A:257:CYS:HA	1:A:286:HIS:HB2	2.00	0.43
1:A:80:ILE:HB	1:A:118:ILE:HG12	2.00	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:330:ASP:O	1:A:331:HIS:C	2.58	0.43
1:A:285:MET:HE3	1:A:318:LEU:HD11	2.01	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: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:124:ASN:OD1	1:A:124:ASN:C	2.58	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:B:86:ILE:HD13	1:B:109:SER:HB3	2.00	0.41
1:A:274:GLU:O	1:A:275:TYR:C	2.59	0.41
1:B:49:VAL:HG22	1:B:82:VAL:HB	2.02	0.41
1:A:334:ARG:HG3	1:A:334:ARG:HH11	1.84	0.41
1:A:257:CYS:HB2	1:A:286:HIS:HB2	2.02	0.41
1:B:137:HIS:CD2	1:B:334:ARG:NH2	2.87	0.41
1:A:24:SER:HG	1:A:326:SER:HB2	1.84	0.41
1:A:335:ILE:HG12	1:A:336:TRP:CG	2.56	0.41
1:A:267:ASN:HB3	1:A:272:MET:HE1	2.02	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:94:GLN:OE1	1:B:184:ASN:ND2	2.48	0.40
1:B:340:THR:HB	1:B:346:GLY:HA2	2.03	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%)	6	8
1	B	345/386 (89%)	306 (89%)	27 (8%)	12 (4%)	4	6
All	All	690/772 (89%)	604 (88%)	64 (9%)	22 (3%)	5	6

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%)	16	30
1	B	288/321 (90%)	273 (95%)	15 (5%)	29	51
All	All	576/642 (90%)	539 (94%)	37 (6%)	22	39

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	11,11,11	1.19	2 (18%)	14,14,14	2.01	3 (21%)

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	-	0/14/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	387	DNO	C3-C2	2.09	1.56	1.53
2	A	387	DNO	C2-C1	2.22	1.54	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	387	DNO	C3-C2-C1	2.19	114.91	111.68
2	A	387	DNO	C5-C4-C3	4.35	119.54	112.47
2	A	387	DNO	C4-C3-C2	4.56	121.53	113.57

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
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, 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	349/386 (90%)	0.42	16 (4%) 36 41	23, 46, 70, 76	0
1	B	349/386 (90%)	0.36	31 (8%) 12 13	22, 41, 65, 95	0
All	All	698/772 (90%)	0.39	47 (6%) 21 23	22, 42, 69, 95	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	GLY	6.3
1	B	293	GLY	6.2
1	B	148	ALA	5.5
1	B	154	LEU	4.5
1	B	383	THR	4.4
1	A	115	ALA	3.9
1	B	339	GLN	3.8
1	A	64	GLU	3.8
1	B	132	THR	3.8
1	A	61	TRP	3.7
1	B	149	PHE	3.6
1	B	152	SER	3.6
1	B	155	ALA	3.6
1	B	159	PRO	3.3
1	B	186	ARG	3.1
1	A	180	ALA	3.0
1	A	286	HIS	2.9
1	B	147	LEU	2.9
1	B	157	VAL	2.9
1	A	378	ALA	2.9
1	B	133	ARG	2.8
1	B	225	TYR	2.8
1	B	150	LEU	2.8
1	B	158	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	111	ARG	2.7
1	A	71	LYS	2.7
1	B	297	PHE	2.6
1	B	292	ALA	2.6
1	B	384	LYS	2.6
1	B	134	SER	2.5
1	B	228	PHE	2.5
1	B	344	GLY	2.5
1	B	183	GLU	2.4
1	A	219	HIS	2.4
1	B	31	LYS	2.4
1	B	30	LYS	2.3
1	A	157	VAL	2.3
1	B	290	VAL	2.3
1	A	60	ALA	2.3
1	A	343	PRO	2.3
1	B	295	TRP	2.2
1	B	187	GLN	2.1
1	B	340	THR	2.1
1	A	118	ILE	2.1
1	A	329	PRO	2.1
1	A	106	TYR	2.0
1	A	59	GLN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MN	A	388	1/1	0.48	0.36	2.04	100,100,100,100	0
2	DNO	A	387	12/12	0.85	0.21	0.16	74,76,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.