



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:50 AM UTC

PDB ID : 3BDK / pdb_00003bdk
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

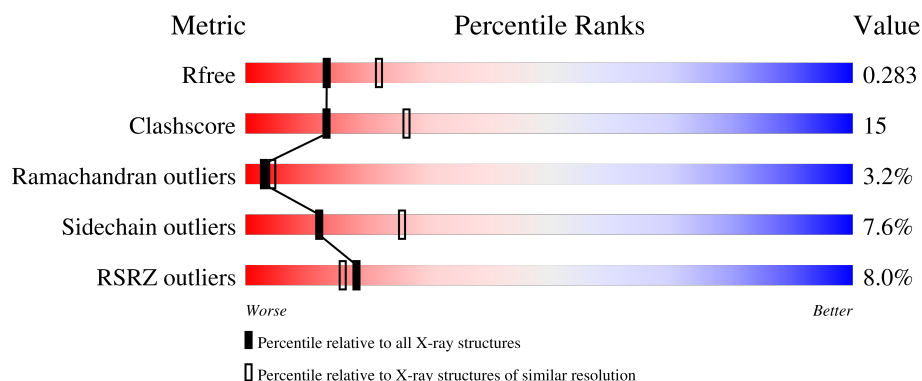
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	8% 60% 25% 5% 10%
1	B	386	7% 62% 24% 5% 10%

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:

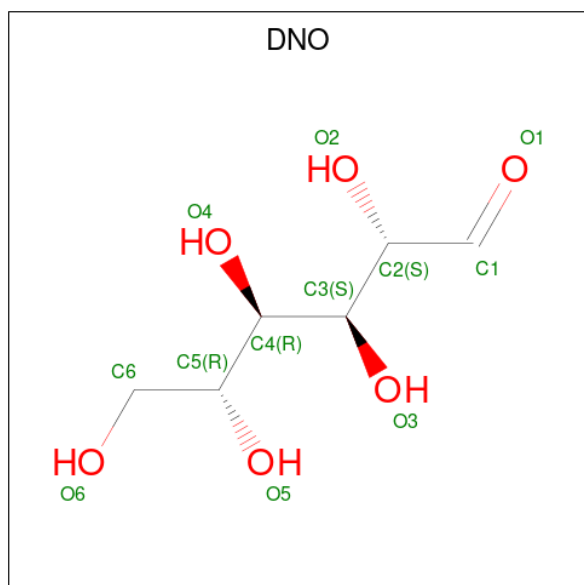
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A4VVI4
A	2	GLY	-	expression tag	UNP A4VVI4
A	3	SER	-	expression tag	UNP A4VVI4
A	4	SER	-	expression tag	UNP A4VVI4
A	5	HIS	-	expression tag	UNP A4VVI4
A	6	HIS	-	expression tag	UNP A4VVI4
A	7	HIS	-	expression tag	UNP A4VVI4
A	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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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 (CCD ID: MN) (formula: Mn).

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

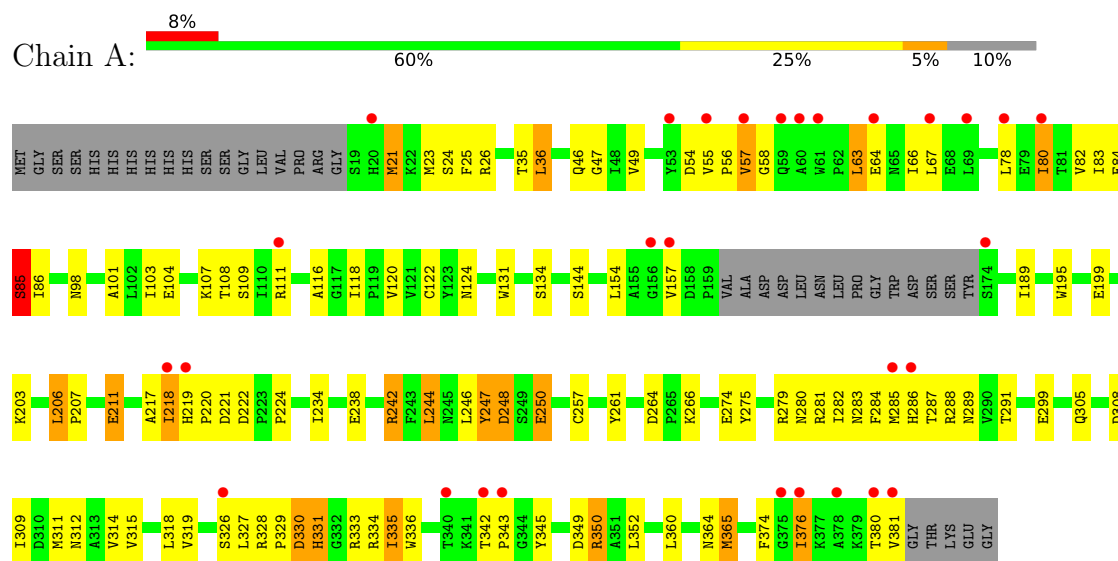
- Molecule 4 is water.

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

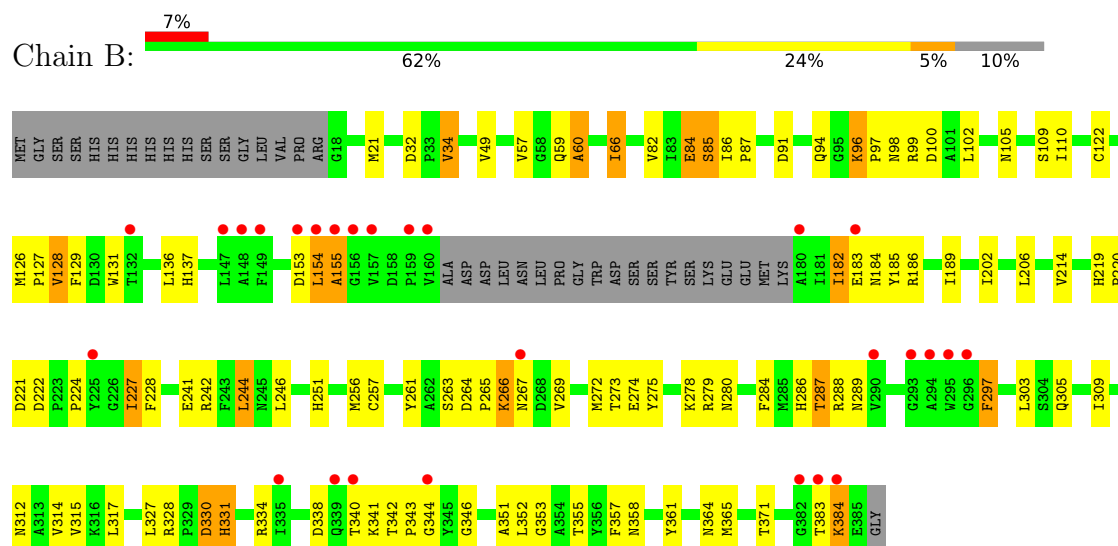
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: D-mannonate dehydratase



• Molecule 1: D-mannonate dehydratase



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 45.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (45.27-2.50) 95.3 (45.27-2.50)	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 (Not available) , 0.283	Depositor DCC
R_{free} test set	1550 reflections (4.87%)	wwPDB-VP
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 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 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, 0.333 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: MN, DNO

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	0.82	1/2805 (0.0%)	0.98	6/3808 (0.2%)
1	B	0.72	0/2800	1.05	8/3802 (0.2%)
All	All	0.77	1/5605 (0.0%)	1.02	14/7610 (0.2%)

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	24.50	2.47	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	THR	CA-C-N	8.89	130.95	119.84
1	B	342	THR	C-N-CA	8.89	130.95	119.84
1	B	96	LYS	CA-C-N	8.49	130.46	119.84
1	B	96	LYS	C-N-CA	8.49	130.46	119.84
1	A	157	VAL	N-CA-C	7.30	119.00	109.58
1	B	297	PHE	N-CA-C	7.06	120.08	108.99
1	A	342	THR	CA-C-N	5.35	126.52	119.84
1	A	342	THR	C-N-CA	5.35	126.52	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	GLU	N-CA-CB	5.16	118.08	110.49
1	A	55	VAL	CA-C-N	5.15	126.28	119.84
1	A	55	VAL	C-N-CA	5.15	126.28	119.84
1	A	380	THR	N-CA-C	5.12	116.85	109.07
1	B	110	ILE	CB-CA-C	-5.06	105.41	111.88
1	B	189	ILE	N-CA-C	5.02	115.56	107.98

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	68	0
2	A	12	0	11	2	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	161	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 (161) 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:319:VAL:HG13	1:A:365:MET:HE3	1.30	1.09
1:A:250:GLU:HG2	1:A:280:ASN:HD22	1.25	1.00
1:A:286:HIS:ND1	1:A:330:ASP:OD2	1.99	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ILE:CD1	1:A:218:ILE:CG1	2.47	0.93
1:A:250:GLU:HG3	1:A:281:ARG:NH1	1.91	0.85
1:A:287:THR:HG23	1:A:287:THR:O	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:A:319:VAL:CG1	1:A:365:MET:HE3	2.11	0.79
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:O	1:B:287:THR:HG23	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	0.71
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:B:214:VAL:O	1:B:251:HIS:HD2	1.75	0.70
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:A:365:MET:HA	1:A:365:MET:HE2	1.81	0.62
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:285:MET:HE2	1:A:318:LEU:HD21	1.82	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:VAL:HG13	1:A:58:GLY:H	1.72	0.55
1:A:286:HIS:CE1	1:A:328:ARG:NH1	2.75	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:O	1:B:287:THR:CG2	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:131:TRP:CD1	2:A:387:DNO:HO4	2.26	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
1:A:131:TRP:CD1	2:A:387:DNO:H1	2.45	0.52
1:A:365:MET:CE	1:A:365:MET:HA	2.38	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:327:LEU:C	1:A:327:LEU:HD23	2.36	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:265:PRO:C	1:B:267:ASN:N	2.70	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:330:ASP:O	1:A:331:HIS:C	2.58	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:A:124:ASN:OD1	1:A:124:ASN:C	2.58	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:274:GLU:O	1:A:275:TYR:C	2.59	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
1:A:352:LEU:HD21	1:B:351:ALA:HB1	1.97	0.45
1:A:218:ILE:HG23	1:A:218:ILE:O	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:57:VAL:CG1	1:A:58:GLY:H	2.29	0.44
1:A:288:ARG:HB2	1:A:330:ASP:HB3	1.99	0.44
1:A:374:PHE:C	1:A:376:ILE:H	2.25	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:A:285:MET:HE2	1:A:318:LEU:HD11	2.00	0.43
1:B:66:ILE:H	1:B:66:ILE:HG12	1.66	0.43
1:B:98:ASN:O	1:B:99:ARG:C	2.61	0.43
1:B:265:PRO:C	1:B:267:ASN:H	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:256:MET:HE3	1:B:273:THR:HA	2.00	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:334:ARG:HH11	1:A:334:ARG:HG3	1.84	0.41
1:B:49:VAL:HG22	1:B:82:VAL:HB	2.02	0.41
1:B:86:ILE:HD13	1:B:109:SER:HB3	2.00	0.41
1:B:265:PRO:O	1:B:266:LYS:C	2.61	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:B:99:ARG:O	1:B:100:ASP:C	2.64	0.41
1:A:335:ILE:HG12	1:A:336:TRP:CG	2.56	0.41
1:A:21:MET:SD	1:A:23:MET:HE1	2.61	0.41
1:A:54:ASP:OD1	1:A:54:ASP:N	2.53	0.41
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:122:CYS:SG	1:A:219:HIS:HB2	2.61	0.41
1:B:154:LEU:O	1:B:155:ALA:C	2.63	0.41
1:A:291:THR:HA	1:A:308:ASP:CG	2.47	0.40
1:B:267:ASN:HB3	1:B:272:MET:HE2	2.02	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%)	3	5
1	B	345/386 (89%)	306 (89%)	27 (8%)	12 (4%)	3	4
All	All	690/772 (89%)	604 (88%)	64 (9%)	22 (3%)	3	4

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
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	265/321 (83%)	242 (91%)	23 (9%)	9	21
1	B	288/321 (90%)	269 (93%)	19 (7%)	15	32
All	All	553/642 (86%)	511 (92%)	42 (8%)	12	26

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	35	THR
1	A	36	LEU
1	A	63	LEU
1	A	64	GLU
1	A	80	ILE
1	A	85	SER
1	A	134	SER
1	A	154	LEU
1	A	189	ILE
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	282	ILE
1	A	305	GLN
1	A	335	ILE
1	A	350	ARG
1	A	365	MET
1	A	376	ILE
1	A	381	VAL
1	B	21	MET
1	B	34	VAL
1	B	66	ILE
1	B	128	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	LEU
1	B	182	ILE
1	B	183	GLU
1	B	206	LEU
1	B	227	ILE
1	B	242	ARG
1	B	244	LEU
1	B	269	VAL
1	B	278	LYS
1	B	280	ASN
1	B	287	THR
1	B	303	LEU
1	B	315	VAL
1	B	328	ARG
1	B	371	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	105	ASN
1	A	188	ASN
1	A	219	HIS
1	A	280	ASN
1	A	283	ASN
1	A	298	GLN
1	A	312	ASN
1	A	324	GLN
1	B	98	ASN
1	B	105	ASN
1	B	137	HIS
1	B	138	HIS
1	B	219	HIS
1	B	237	GLN
1	B	251	HIS
1	B	286	HIS
1	B	298	GLN
1	B	305	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 oligosaccharides 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	1.13	1 (10%)	13,14,14	2.02	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	-	10/15/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	387	DNO	C3-C2	2.17	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	387	DNO	C5-C4-C3	4.60	119.54	112.48
2	A	387	DNO	C4-C3-C2	4.59	121.53	113.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	387	DNO	O1-C1-C2-C3
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	C3-C4-C5-O5
2	A	387	DNO	C2-C3-C4-O4
2	A	387	DNO	O3-C3-C4-C5
2	A	387	DNO	O4-C4-C5-C6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	387	DNO	2	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%)	0.66	29 (8%) 17 15	23, 46, 70, 76	0
1	B	349/386 (90%)	0.54	27 (7%) 19 17	22, 41, 65, 95	0
All	All	698/772 (90%)	0.60	56 (8%) 18 16	22, 42, 69, 95	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	GLY	5.1
1	A	174	SER	4.6
1	B	383	THR	4.4
1	A	343	PRO	4.1
1	B	384	LYS	4.1
1	B	148	ALA	4.0
1	B	154	LEU	3.7
1	B	160	VAL	3.6
1	B	157	VAL	3.6
1	B	340	THR	3.4
1	A	340	THR	3.3
1	A	286	HIS	3.2
1	A	380	THR	3.1
1	A	69	LEU	3.1
1	A	378	ALA	3.0
1	B	155	ALA	3.0
1	A	80	ILE	2.9
1	A	219	HIS	2.9
1	A	57	VAL	2.8
1	A	157	VAL	2.8
1	B	225	TYR	2.8
1	A	381	VAL	2.8
1	B	344	GLY	2.7
1	A	375	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	153	ASP	2.7
1	A	64	GLU	2.7
1	B	290	VAL	2.6
1	B	295	TRP	2.6
1	B	183	GLU	2.6
1	B	180	ALA	2.5
1	B	156	GLY	2.5
1	A	53	TYR	2.5
1	A	342	THR	2.5
1	B	296	GLY	2.4
1	B	267	ASN	2.4
1	B	335	ILE	2.4
1	A	78	LEU	2.4
1	A	55	VAL	2.3
1	B	132	THR	2.3
1	B	339	GLN	2.3
1	A	60	ALA	2.3
1	A	156	GLY	2.3
1	A	376	ILE	2.3
1	A	67	LEU	2.2
1	B	147	LEU	2.2
1	B	382	GLY	2.2
1	B	294	ALA	2.2
1	A	59	GLN	2.2
1	A	326	SER	2.2
1	A	218	ILE	2.1
1	A	61	TRP	2.1
1	A	111	ARG	2.1
1	A	285	MET	2.1
1	A	20	HIS	2.1
1	B	149	PHE	2.0
1	B	159	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MN	A	388	1/1	0.70	0.24	100,100,100,100	0
2	DNO	A	387	12/12	0.74	0.17	74,76,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.