



Full wwPDB X-ray Structure Validation Report

May 30, 2014 – 02:41 AM EDT

PDB ID : 4ONQ
Title : Crystal structure of ntDRM E283S/R309S/F310S/Y590S/D591Smutant
Authors : Du, J.; Patel, D.J.
Deposited on : 2014-01-28
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

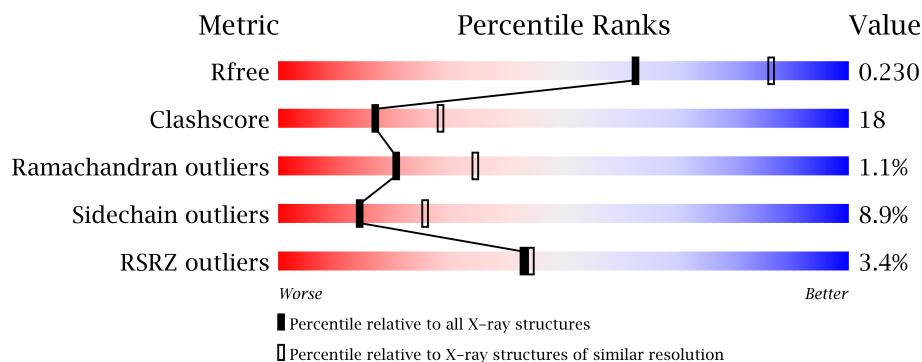
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SFG	A	700	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5301 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

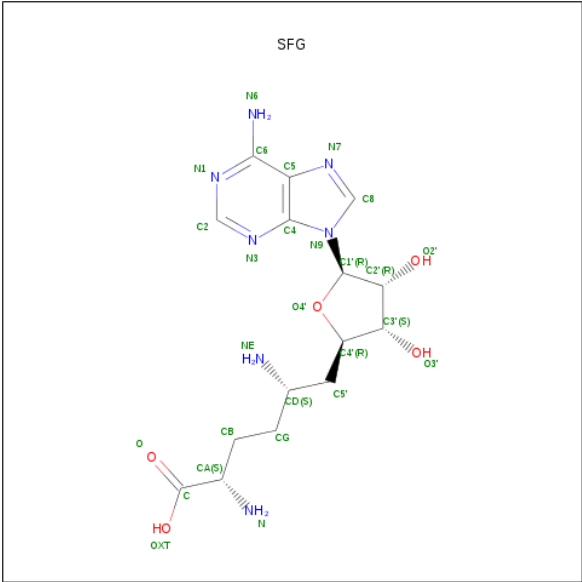
- Molecule 1 is a protein called DNA methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2603	1676	454	465	8			
1	B	317	Total	C	N	O	S	0	0	0
			2531	1630	441	453	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	SER	GLU	ENGINEERED MUTATION	UNP Q76KU6
A	309	SER	ARG	ENGINEERED MUTATION	UNP Q76KU6
A	310	SER	PHE	ENGINEERED MUTATION	UNP Q76KU6
A	590	SER	TYR	ENGINEERED MUTATION	UNP Q76KU6
A	591	SER	ASP	ENGINEERED MUTATION	UNP Q76KU6
B	283	SER	GLU	ENGINEERED MUTATION	UNP Q76KU6
B	309	SER	ARG	ENGINEERED MUTATION	UNP Q76KU6
B	310	SER	PHE	ENGINEERED MUTATION	UNP Q76KU6
B	590	SER	TYR	ENGINEERED MUTATION	UNP Q76KU6
B	591	SER	ASP	ENGINEERED MUTATION	UNP Q76KU6

- Molecule 2 is SINEFUNGIN (three-letter code: SFG) (formula: C₁₅H₂₃N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		
2	B	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	39	Total	O	0	0
			39	39		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	131.50Å 131.50Å 88.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.88 – 2.50 43.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.88-2.50) 99.9 (43.04-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.185 , 0.230 0.182 , 0.230	Depositor DCC
R_{free} test set	1525 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 30042 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5301	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SFG

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	0.69	1/2673 (0.0%)	0.58	0/3632
1	B	0.74	2/2597 (0.1%)	0.64	0/3525
All	All	0.72	3/5270 (0.1%)	0.61	0/7157

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	PRO	N-CD	-5.93	1.39	1.47
1	A	525	TRP	NE1-CE2	-5.07	1.30	1.37
1	B	593	VAL	CA-CB	-5.01	1.44	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts i

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2603	0	2607	37	0
1	B	2531	0	2528	146	0
2	A	27	0	22	3	0
2	B	27	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	74	0	0	1	0
3	B	39	0	0	1	0
All	All	5301	0	5179	183	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (183) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:LEU:CD2	1:B:285:ALA:HB3	1.25	1.58
1:B:352:THR:CG2	1:B:355:GLU:HG3	1.42	1.45
1:A:261:LYS:HG2	1:A:262:PRO:CD	1.57	1.34
1:B:281:LEU:HD21	1:B:285:ALA:CB	1.56	1.34
1:B:300:PRO:O	1:B:303:VAL:HG23	1.34	1.27
1:B:281:LEU:HD23	1:B:282:PRO:CD	1.63	1.25
1:B:352:THR:HG22	1:B:355:GLU:CG	1.67	1.23
1:A:261:LYS:CG	1:A:262:PRO:HD3	1.69	1.22
1:B:281:LEU:HD23	1:B:282:PRO:N	1.56	1.21
1:B:352:THR:CG2	1:B:355:GLU:CG	2.22	1.17
1:B:258:ARG:HH21	1:B:258:ARG:CG	1.58	1.14
1:B:352:THR:HG21	1:B:355:GLU:HG3	1.23	1.11
1:B:298:LEU:HD22	1:B:298:LEU:N	1.65	1.11
1:B:352:THR:HG23	1:B:355:GLU:H	1.16	1.11
1:B:281:LEU:CD1	1:B:285:ALA:HB1	1.83	1.07
1:B:300:PRO:HD2	1:B:303:VAL:CG2	1.84	1.07
1:B:281:LEU:HD11	1:B:285:ALA:HB1	1.09	1.06
1:A:352:THR:OG1	1:A:355:GLU:HG3	1.55	1.06
1:B:281:LEU:CD2	1:B:285:ALA:CB	2.21	1.04
1:B:281:LEU:HD11	1:B:285:ALA:CB	1.87	1.03
1:A:286:VAL:HG22	1:A:287:GLY:H	1.19	1.02
1:B:300:PRO:HD2	1:B:303:VAL:HG21	1.03	1.02
1:B:298:LEU:CD2	1:B:298:LEU:H	1.74	1.00
1:B:258:ARG:HG2	1:B:258:ARG:NH2	1.41	0.98
1:B:300:PRO:CD	1:B:303:VAL:HG21	1.95	0.96
1:B:281:LEU:HD22	1:B:285:ALA:HB3	1.44	0.96
1:B:281:LEU:CD2	1:B:282:PRO:CD	2.44	0.95
1:B:281:LEU:CD1	1:B:285:ALA:CB	2.44	0.92
1:B:281:LEU:CD2	1:B:282:PRO:HD2	2.01	0.90
1:B:315:GLU:HG2	1:B:315:GLU:O	1.71	0.89
1:B:266:PHE:HD2	1:B:339:VAL:HG21	1.36	0.89
1:B:281:LEU:HD23	1:B:282:PRO:HD2	1.55	0.87
1:B:396:PHE:CE1	1:B:401:PRO:CD	2.58	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:268:VAL:HB	1:B:269:PRO:HD2	1.55	0.86
1:B:298:LEU:CD2	1:B:298:LEU:N	2.30	0.85
1:B:266:PHE:CD2	1:B:339:VAL:HG21	2.10	0.85
1:A:271:GLU:HB3	1:A:272:PRO:HD2	1.60	0.84
1:B:281:LEU:CG	1:B:285:ALA:HB3	2.09	0.83
1:B:540:VAL:HG13	1:B:595:ILE:HD11	1.60	0.83
1:B:281:LEU:HD23	1:B:282:PRO:CG	2.09	0.83
1:B:281:LEU:CG	1:B:282:PRO:HD2	2.10	0.82
1:B:396:PHE:CD1	1:B:401:PRO:HD3	2.15	0.82
1:B:352:THR:HG23	1:B:355:GLU:N	1.95	0.81
1:B:396:PHE:CE1	1:B:401:PRO:HD3	2.16	0.81
1:B:281:LEU:HD13	1:B:285:ALA:O	1.81	0.80
1:B:352:THR:HG22	1:B:355:GLU:CB	2.11	0.80
1:B:261:LYS:HB2	1:B:262:PRO:HD3	1.62	0.79
1:B:281:LEU:HD21	1:B:285:ALA:HB3	0.80	0.79
1:B:258:ARG:NH2	1:B:258:ARG:N	2.30	0.79
1:A:352:THR:OG1	1:A:355:GLU:CG	2.32	0.78
1:B:300:PRO:CD	1:B:303:VAL:CG2	2.58	0.78
1:B:281:LEU:HD11	1:B:314:ILE:HD11	1.64	0.78
1:B:281:LEU:HG	1:B:282:PRO:HD2	1.66	0.77
1:A:286:VAL:HG22	1:A:287:GLY:N	2.00	0.75
1:A:300:PRO:HG2	1:A:303:VAL:HG23	1.69	0.75
1:B:298:LEU:H	1:B:298:LEU:HD22	1.34	0.72
1:B:352:THR:HG22	1:B:355:GLU:CD	2.09	0.71
1:B:322:LYS:HB2	1:B:372:LYS:HE3	1.74	0.69
1:B:543:LEU:HD12	1:B:595:ILE:HD13	1.75	0.68
1:B:258:ARG:HD3	1:B:301:LYS:CD	2.22	0.68
1:B:258:ARG:HG3	1:B:259:LEU:CD1	2.24	0.68
1:B:444:THR:O	1:B:454:ARG:HD3	1.95	0.67
1:A:261:LYS:CG	1:A:262:PRO:CD	2.48	0.67
1:B:258:ARG:HH21	1:B:258:ARG:HG2	0.65	0.66
1:A:269:PRO:HA	1:B:346:PHE:HZ	1.59	0.66
1:B:268:VAL:HB	1:B:269:PRO:CD	2.24	0.65
1:B:298:LEU:H	1:B:298:LEU:HD23	1.60	0.65
1:B:281:LEU:CD2	1:B:282:PRO:HG2	2.27	0.64
1:B:540:VAL:CG1	1:B:540:VAL:O	2.45	0.64
1:A:283:SER:O	1:A:286:VAL:HG12	1.97	0.63
1:B:258:ARG:HH21	1:B:258:ARG:N	1.92	0.63
1:A:444:THR:O	1:A:454:ARG:HD3	1.98	0.62
1:B:281:LEU:CD1	1:B:314:ILE:HD11	2.29	0.62
1:B:266:PHE:HD2	1:B:339:VAL:CG2	2.10	0.62
1:B:377:GLN:N	1:B:377:GLN:OE1	2.25	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:LEU:CD2	1:B:282:PRO:CG	2.76	0.61
1:B:390:ARG:O	1:B:394:GLU:HB2	2.00	0.61
1:B:540:VAL:HG13	1:B:595:ILE:CD1	2.31	0.61
1:B:307:ILE:HD12	1:B:589:PHE:CE1	2.35	0.61
1:B:307:ILE:HD12	1:B:589:PHE:CZ	2.36	0.60
1:A:346:PHE:CG	1:A:347:PRO:HA	2.35	0.60
1:B:352:THR:HG22	1:B:355:GLU:HB2	1.83	0.60
1:B:258:ARG:HG3	1:B:259:LEU:HD12	1.84	0.60
1:A:261:LYS:HG2	1:A:262:PRO:HD3	0.73	0.60
1:B:281:LEU:CD2	1:B:282:PRO:N	2.48	0.60
1:B:552:ILE:HD12	1:B:557:GLY:HA2	1.84	0.60
1:B:263:MET:HG2	1:B:319:VAL:HA	1.84	0.59
1:B:302:GLY:O	1:B:306:THR:OG1	2.20	0.59
1:B:268:VAL:CB	1:B:269:PRO:HD2	2.29	0.59
1:B:307:ILE:CD1	1:B:589:PHE:CZ	2.86	0.58
1:B:511:VAL:HG12	2:B:700:SFG:H2	1.83	0.58
1:B:352:THR:CG2	1:B:355:GLU:CB	2.75	0.58
1:B:281:LEU:CG	1:B:285:ALA:CB	2.77	0.58
1:B:281:LEU:HD21	1:B:282:PRO:HG2	1.86	0.57
1:B:281:LEU:HD23	1:B:281:LEU:C	2.23	0.57
1:B:363:TRP:O	1:B:365:PRO:HD3	2.04	0.57
1:B:281:LEU:HD21	1:B:285:ALA:HB2	1.75	0.55
1:B:299:ALA:HB1	1:B:300:PRO:CD	2.36	0.55
1:A:285:ALA:HB1	1:A:314:ILE:HD11	1.89	0.55
1:B:258:ARG:HD3	1:B:301:LYS:CE	2.36	0.55
1:B:540:VAL:O	1:B:540:VAL:HG12	2.04	0.55
1:B:258:ARG:CG	1:B:258:ARG:NH2	2.30	0.54
1:B:550:GLN:O	1:B:554:SER:OG	2.25	0.54
1:B:299:ALA:HB1	1:B:300:PRO:HD2	1.89	0.54
1:B:300:PRO:O	1:B:303:VAL:CG2	2.30	0.53
1:B:300:PRO:O	1:B:303:VAL:N	2.41	0.53
1:B:549:GLU:HB3	1:B:602:ILE:HD13	1.92	0.52
1:A:286:VAL:CG2	1:A:287:GLY:H	2.02	0.52
1:B:258:ARG:NE	1:B:301:LYS:HD3	2.25	0.52
1:A:550:GLN:HA	1:A:553:GLU:HG2	1.93	0.51
1:B:263:MET:O	1:B:319:VAL:HA	2.10	0.51
1:B:396:PHE:CE1	1:B:401:PRO:HD2	2.44	0.51
1:B:281:LEU:CD1	1:B:314:ILE:CD1	2.89	0.51
1:B:307:ILE:HG22	1:B:334:ILE:HD12	1.93	0.51
1:B:354:HIS:CE1	1:B:361:LYS:HA	2.46	0.50
1:B:540:VAL:HG11	1:B:591:SER:HB3	1.94	0.49
1:B:258:ARG:CD	1:B:301:LYS:CD	2.89	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:591:SER:HA	1:B:594:ARG:HG2	1.93	0.49
1:B:539:ASP:OD1	1:B:541:GLN:OE1	2.31	0.49
1:B:435:MET:HE2	1:B:436:LEU:HA	1.94	0.48
1:B:488:PHE:O	2:B:700:SFG:HG1	2.13	0.48
1:B:264:ILE:HD12	1:B:323:TYR:CE2	2.48	0.48
1:A:488:PHE:HB3	2:A:700:SFG:H5'2	1.96	0.47
1:B:261:LYS:HB2	1:B:262:PRO:CD	2.39	0.47
1:B:268:VAL:CB	1:B:269:PRO:CD	2.89	0.47
1:A:539:ASP:O	1:A:542:GLN:HG2	2.13	0.47
1:B:548:LEU:O	1:B:552:ILE:HG12	2.15	0.47
2:B:700:SFG:HG2	2:B:700:SFG:H4'	1.64	0.47
1:A:378:THR:HG22	1:A:456:LYS:HA	1.97	0.47
1:A:397:ASP:OD1	1:A:397:ASP:N	2.23	0.47
1:B:258:ARG:HD3	1:B:301:LYS:HD2	1.94	0.46
1:A:490:GLY:HA3	2:A:700:SFG:HA	1.98	0.46
1:A:286:VAL:HG13	1:A:287:GLY:N	2.30	0.46
1:A:328:ALA:O	1:A:375:CYS:HA	2.16	0.46
1:B:539:ASP:OD1	1:B:540:VAL:N	2.48	0.46
1:B:396:PHE:CD1	1:B:401:PRO:CD	2.90	0.46
1:B:396:PHE:CE1	1:B:401:PRO:CG	2.98	0.46
1:B:594:ARG:O	1:B:598:LEU:HD13	2.16	0.46
1:A:346:PHE:CD2	1:A:347:PRO:HA	2.51	0.45
1:B:281:LEU:HD23	1:B:282:PRO:CA	2.41	0.45
1:B:300:PRO:CG	1:B:303:VAL:CG2	2.94	0.45
1:B:268:VAL:HG23	1:B:271:GLU:H	1.80	0.45
1:B:364:TRP:HA	1:B:365:PRO:HD2	1.86	0.45
1:B:263:MET:HE3	1:B:320:ASP:HB2	1.98	0.45
1:B:264:ILE:HG13	1:B:268:VAL:HG13	1.98	0.45
1:B:263:MET:HE1	1:B:330:LYS:HG2	1.98	0.45
1:B:284:GLN:CD	1:B:284:GLN:H	2.20	0.45
1:B:307:ILE:HD13	1:B:589:PHE:CZ	2.52	0.45
1:B:307:ILE:HD13	1:B:589:PHE:CE2	2.52	0.45
1:B:300:PRO:C	1:B:303:VAL:HG23	2.24	0.45
1:B:315:GLU:CG	1:B:315:GLU:O	2.54	0.44
1:A:404:VAL:O	1:A:408:VAL:HG13	2.18	0.44
1:A:271:GLU:HB3	1:A:272:PRO:CD	2.40	0.44
1:B:601:SER:OG	1:B:602:ILE:N	2.51	0.44
1:A:277:VAL:HG12	1:A:277:VAL:O	2.17	0.44
1:B:258:ARG:HE	1:B:301:LYS:HD3	1.82	0.43
1:B:281:LEU:HD12	1:B:314:ILE:CD1	2.48	0.43
1:B:505:LEU:O	3:B:809:HOH:O	2.21	0.43
1:B:263:MET:HB3	1:B:263:MET:HE3	1.55	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:451:ARG:O	1:A:454:ARG:HB2	2.18	0.43
1:B:321:SER:HB2	1:B:329:ARG:HB3	2.00	0.43
1:B:340:GLU:OE2	1:B:340:GLU:N	2.52	0.43
1:A:270:THR:O	1:A:270:THR:OG1	2.38	0.42
1:A:490:GLY:O	1:A:517:ASN:HB3	2.20	0.42
1:B:287:GLY:HA3	1:B:288:PRO:HD3	1.93	0.42
1:A:398:GLY:HA2	1:A:399:GLU:HA	1.67	0.42
1:A:550:GLN:HA	1:A:553:GLU:OE2	2.20	0.42
1:B:307:ILE:HG23	1:B:307:ILE:HD12	1.87	0.42
1:A:269:PRO:CA	1:B:346:PHE:HZ	2.29	0.42
1:A:489:SER:OG	1:A:510:SER:OG	2.24	0.42
1:B:346:PHE:CD1	1:B:347:PRO:HA	2.55	0.41
2:A:700:SFG:H4'	2:A:700:SFG:HG2	1.34	0.41
1:B:263:MET:O	1:B:263:MET:HG2	2.20	0.41
1:B:281:LEU:CD2	1:B:281:LEU:C	2.87	0.41
1:A:294:GLU:OE2	3:A:858:HOH:O	2.22	0.41
1:B:288:PRO:HA	1:B:289:PRO:HA	1.63	0.41
1:B:390:ARG:HG3	1:B:391:LYS:N	2.36	0.41
1:B:294:GLU:HG3	1:B:333:TYR:CE1	2.56	0.41
1:B:449:ILE:HD12	1:B:516:VAL:HG13	2.02	0.41
1:A:298:LEU:HD13	1:A:298:LEU:HA	1.82	0.40
1:B:552:ILE:HG23	1:B:557:GLY:HA2	2.03	0.40
1:B:258:ARG:O	1:B:259:LEU:HB2	2.19	0.40
1:B:522:ARG:CZ	1:B:534:LEU:HD23	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	323/357 (90%)	315 (98%)	4 (1%)	4 (1%)	19	32
1	B	311/357 (87%)	296 (95%)	12 (4%)	3 (1%)	22	38
All	All	634/714 (89%)	611 (96%)	16 (2%)	7 (1%)	21	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	GLY
1	A	262	PRO
1	B	288	PRO
1	A	565	SER
1	B	259	LEU
1	B	260	PRO
1	A	286	VAL

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	286/312 (92%)	266 (93%)	20 (7%)	21	38
1	B	277/312 (89%)	247 (89%)	30 (11%)	9	17
All	All	563/624 (90%)	513 (91%)	50 (9%)	14	26

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ARG
1	A	259	LEU
1	A	261	LYS
1	A	270	THR
1	A	281	LEU
1	A	319	VAL
1	A	345	LEU
1	A	355	GLU
1	A	357	LEU
1	A	360	SER
1	A	377	GLN
1	A	382	SER
1	A	384	GLN
1	A	404	VAL
1	A	435	MET
1	A	507	THR
1	A	544	ASN

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Mol	Chain	Res	Type
1	A	548	LEU
1	A	551	LEU
1	A	561	VAL
1	B	258	ARG
1	B	263	MET
1	B	270	THR
1	B	279	ARG
1	B	294	GLU
1	B	298	LEU
1	B	301	LYS
1	B	303	VAL
1	B	306	THR
1	B	311	LEU
1	B	313	ASP
1	B	315	GLU
1	B	345	LEU
1	B	359	LEU
1	B	390	ARG
1	B	417	LEU
1	B	420	VAL
1	B	435	MET
1	B	451	ARG
1	B	516	VAL
1	B	546	ASP
1	B	547	ARG
1	B	548	LEU
1	B	551	LEU
1	B	554	SER
1	B	565	SER
1	B	590	SER
1	B	591	SER
1	B	597	ASP
1	B	601	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	GLN
1	A	506	ASN
1	A	541	GLN
1	B	335	HIS
1	B	354	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 ligands are modelled in this entry.

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	SFG	A	700	-	29,29,29	1.68	7 (24%)	42,42,42	6.12	17 (40%)
2	SFG	B	700	-	29,29,29	1.48	3 (10%)	42,42,42	2.33	11 (26%)

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	SFG	A	700	-	-	0/17/33/33	0/3/3/3
2	SFG	B	700	-	-	0/17/33/33	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	SFG	C4-N9	-4.64	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	SFG	C2-N3	4.58	1.40	1.32
2	A	700	SFG	C2-N1	3.07	1.39	1.33
2	A	700	SFG	C5-C4	-2.98	1.33	1.40
2	B	700	SFG	OXT-C	-2.73	1.20	1.30
2	A	700	SFG	C8-N9	-2.62	1.32	1.36
2	A	700	SFG	O4'-C4'	2.43	1.50	1.45
2	B	700	SFG	C8-N9	-2.42	1.33	1.36
2	A	700	SFG	C4-N9	-2.39	1.34	1.37
2	A	700	SFG	O4'-C1'	2.17	1.43	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	SFG	O4'-C1'-C2'	-20.19	77.30	106.69
2	A	700	SFG	O4'-C4'-C5'	-19.26	80.46	109.44
2	A	700	SFG	C5'-C4'-C3'	17.25	134.63	115.19
2	A	700	SFG	N3-C2-N1	-12.27	118.10	128.89
2	A	700	SFG	C4'-C5'-CD	-8.93	97.37	113.46
2	A	700	SFG	O4'-C4'-C3'	-8.14	88.61	105.16
2	A	700	SFG	C3'-C2'-C1'	-7.30	89.48	100.92
2	B	700	SFG	N3-C2-N1	-6.98	122.75	128.89
2	B	700	SFG	C5-C4-N3	-6.89	119.26	125.98
2	A	700	SFG	C5-C4-N3	-6.10	120.03	125.98
2	B	700	SFG	N3-C4-N9	5.09	134.12	125.39
2	A	700	SFG	C5'-CD-CG	-3.65	100.28	114.16
2	B	700	SFG	C5'-C4'-C3'	-3.61	111.12	115.19
2	A	700	SFG	N3-C4-N9	3.48	131.36	125.39
2	B	700	SFG	C4-C5-N7	-3.39	106.14	109.41
2	B	700	SFG	C8-N9-C4	3.25	109.60	106.96
2	B	700	SFG	C4'-O4'-C1'	-3.14	106.27	109.72
2	A	700	SFG	C1'-N9-C4	-3.07	121.33	126.64
2	A	700	SFG	CG-CB-CA	-2.97	103.53	113.89
2	B	700	SFG	C2-N3-C4	2.95	121.76	113.27
2	A	700	SFG	C4'-O4'-C1'	-2.80	106.64	109.72
2	A	700	SFG	C6-C5-C4	2.79	120.68	117.55
2	B	700	SFG	C1'-N9-C4	-2.55	122.22	126.64
2	A	700	SFG	C8-N9-C1'	2.50	130.86	126.15
2	A	700	SFG	C2-N3-C4	2.47	120.39	113.27
2	B	700	SFG	O4'-C1'-C2'	-2.38	103.23	106.69
2	A	700	SFG	C4-C5-N7	-2.33	107.16	109.41
2	B	700	SFG	C4'-C5'-CD	-2.18	109.54	113.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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(Å ²)	Q<0.9
1	A	327/357 (91%)	0.01	8 (2%) 56 58	27, 50, 95, 157	0
1	B	317/357 (88%)	0.15	13 (4%) 35 36	32, 65, 114, 165	0
All	All	644/714 (90%)	0.08	21 (3%) 43 45	27, 57, 107, 165	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	3.9
1	B	261	LYS	3.6
1	B	315	GLU	3.1
1	B	396	PHE	3.0
1	B	595	ILE	2.9
1	A	398	GLY	2.7
1	A	277	VAL	2.7
1	A	259	LEU	2.6
1	B	283	SER	2.5
1	B	259	LEU	2.4
1	B	302	GLY	2.3
1	B	284	GLN	2.3
1	A	566	PRO	2.2
1	A	261	LYS	2.2
1	A	301	LYS	2.1
1	B	346	PHE	2.1
1	A	285	ALA	2.1
1	A	397	ASP	2.1
1	B	293	TYR	2.0
1	B	318	PHE	2.0
1	B	555	PHE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SFG	A	700	27/27	0.24	2.15	66,86,99,102	0
2	SFG	B	700	27/27	0.18	0.92	72,83,93,95	0

6.5 Other polymers

There are no such residues in this entry.