



Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2014 – 05:12 AM EDT

PDB ID : 3WIE
Title : Structure of a glucose dehydrogenase T277F mutant in complex with D-glucose and NAADP
Authors : Sakuraba, H.; Kanoh, Y.; Yoneda, K; Ohshima, T
Deposited on : 2013-09-10
Resolution : 2.33 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>

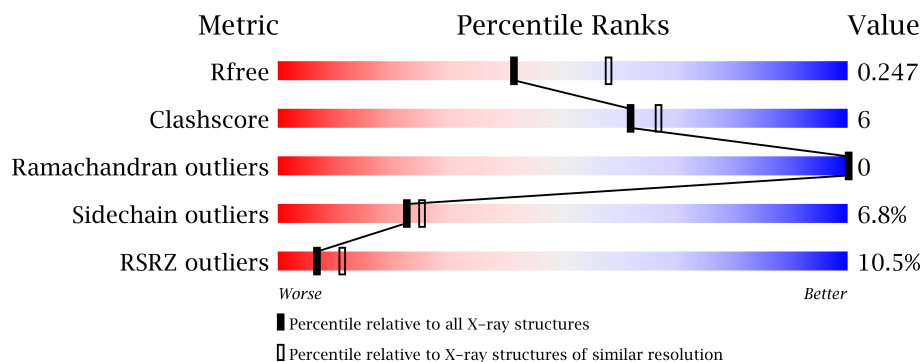
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
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) : stable22978

1 Overall quality at a glance





The reported resolution of this entry is 2.33 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	4049 (2.38-2.30)
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

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	369	
1	B	369	
1	C	369	
1	D	369	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11772 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 Glucose 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	B	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	C	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	D	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	PHE	THR	ENGINEERED MUTATION	UNP Q979W2
A	362	LEU	-	EXPRESSION TAG	UNP Q979W2
A	363	GLU	-	EXPRESSION TAG	UNP Q979W2
A	364	HIS	-	EXPRESSION TAG	UNP Q979W2
A	365	HIS	-	EXPRESSION TAG	UNP Q979W2
A	366	HIS	-	EXPRESSION TAG	UNP Q979W2
A	367	HIS	-	EXPRESSION TAG	UNP Q979W2
A	368	HIS	-	EXPRESSION TAG	UNP Q979W2
A	369	HIS	-	EXPRESSION TAG	UNP Q979W2
B	277	PHE	THR	ENGINEERED MUTATION	UNP Q979W2
B	362	LEU	-	EXPRESSION TAG	UNP Q979W2
B	363	GLU	-	EXPRESSION TAG	UNP Q979W2
B	364	HIS	-	EXPRESSION TAG	UNP Q979W2
B	365	HIS	-	EXPRESSION TAG	UNP Q979W2
B	366	HIS	-	EXPRESSION TAG	UNP Q979W2
B	367	HIS	-	EXPRESSION TAG	UNP Q979W2
B	368	HIS	-	EXPRESSION TAG	UNP Q979W2
B	369	HIS	-	EXPRESSION TAG	UNP Q979W2
C	277	PHE	THR	ENGINEERED MUTATION	UNP Q979W2
C	362	LEU	-	EXPRESSION TAG	UNP Q979W2
C	363	GLU	-	EXPRESSION TAG	UNP Q979W2

Continued on next page...

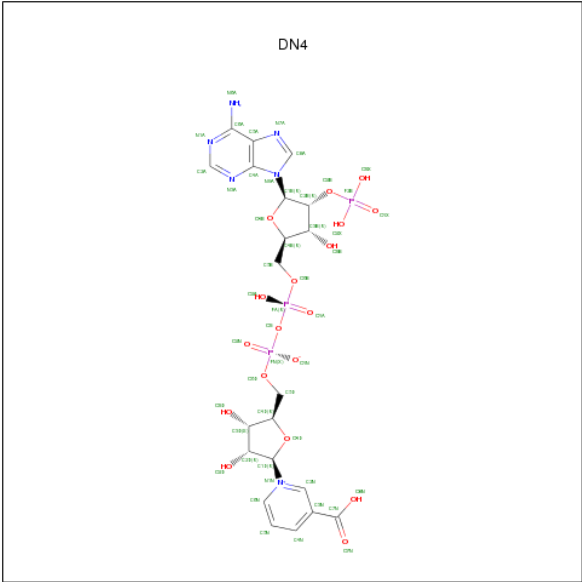
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	364	HIS	-	EXPRESSION TAG	UNP Q979W2
C	365	HIS	-	EXPRESSION TAG	UNP Q979W2
C	366	HIS	-	EXPRESSION TAG	UNP Q979W2
C	367	HIS	-	EXPRESSION TAG	UNP Q979W2
C	368	HIS	-	EXPRESSION TAG	UNP Q979W2
C	369	HIS	-	EXPRESSION TAG	UNP Q979W2
D	277	PHE	THR	ENGINEERED MUTATION	UNP Q979W2
D	362	LEU	-	EXPRESSION TAG	UNP Q979W2
D	363	GLU	-	EXPRESSION TAG	UNP Q979W2
D	364	HIS	-	EXPRESSION TAG	UNP Q979W2
D	365	HIS	-	EXPRESSION TAG	UNP Q979W2
D	366	HIS	-	EXPRESSION TAG	UNP Q979W2
D	367	HIS	-	EXPRESSION TAG	UNP Q979W2
D	368	HIS	-	EXPRESSION TAG	UNP Q979W2
D	369	HIS	-	EXPRESSION TAG	UNP Q979W2

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

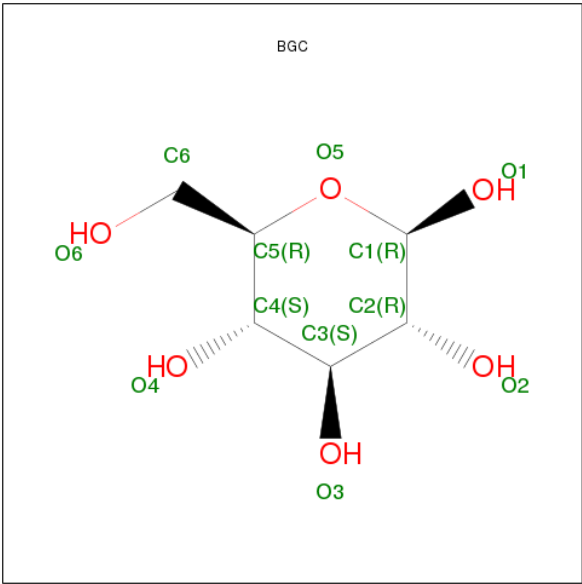
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0

- Molecule 3 is [[(2R,3R,4R,5R)-5-(6-AMINOPURIN-9-YL)-3-OXIDANYL-4-PHOSPHONOXY-OXOLAN-2-YL]METHOXY-OXIDANYL-PHOSPHORYL][(2R,3S,4R,5R)-5-(3-CARBOXYPYRIDIN-1-IUM-1-YL)-3,4-BIS(OXIDANYL)OXOLAN-2-YL]METHYLPHOSPHATE (three-letter code: DN4) (formula: C₂₁H₂₇N₆O₁₈P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	6	18	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	6	18	3		

- Molecule 4 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0
4	B	1	Total C O 12 6 6	0	0
4	C	1	Total C O 12 6 6	0	0
4	D	1	Total C O 12 6 6	0	0

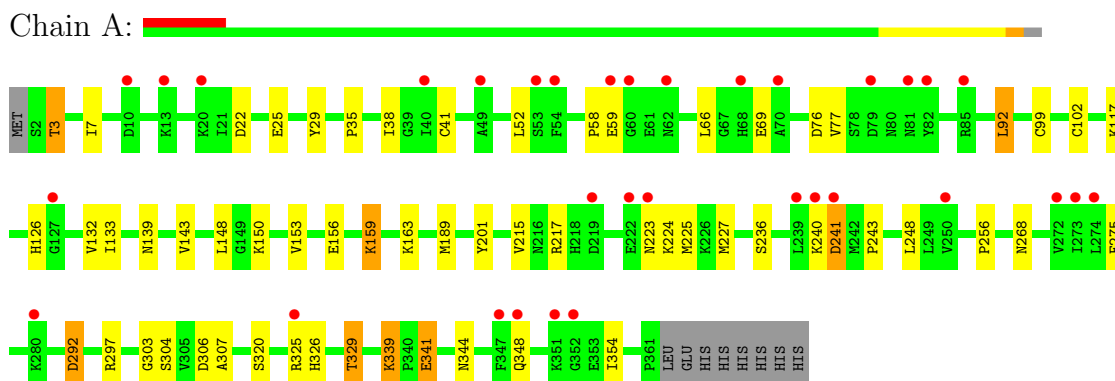
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	60	Total O 60 60	0	0
5	B	61	Total O 61 61	0	0
5	C	51	Total O 51 51	0	0
5	D	44	Total O 44 44	0	0

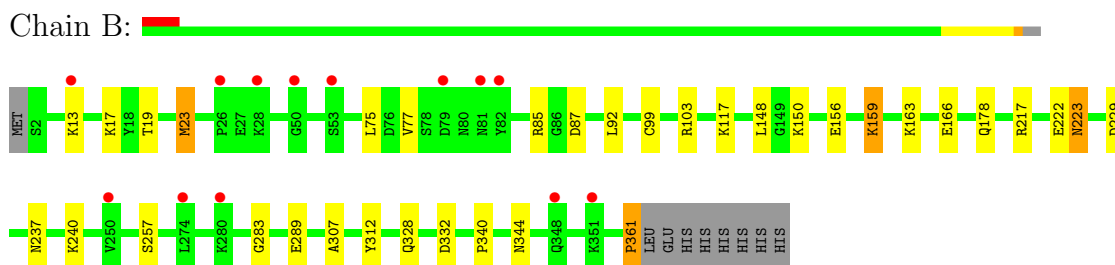
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

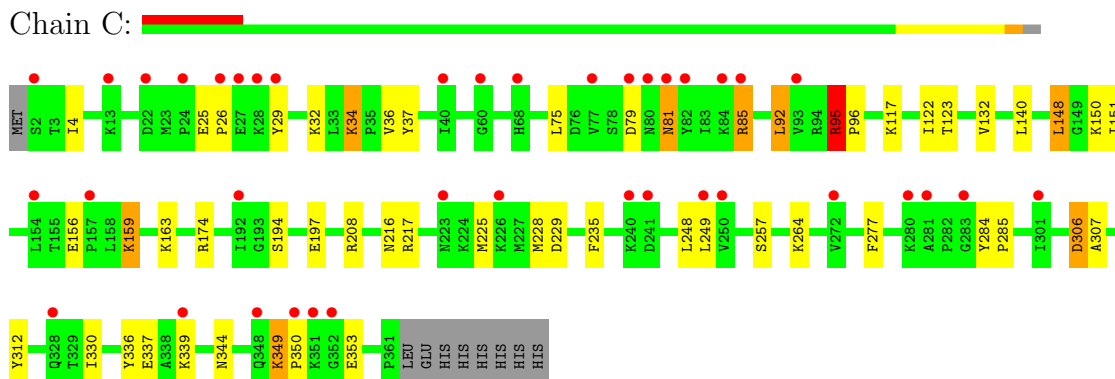
- Molecule 1: Glucose 1-dehydrogenase



- Molecule 1: Glucose 1-dehydrogenase

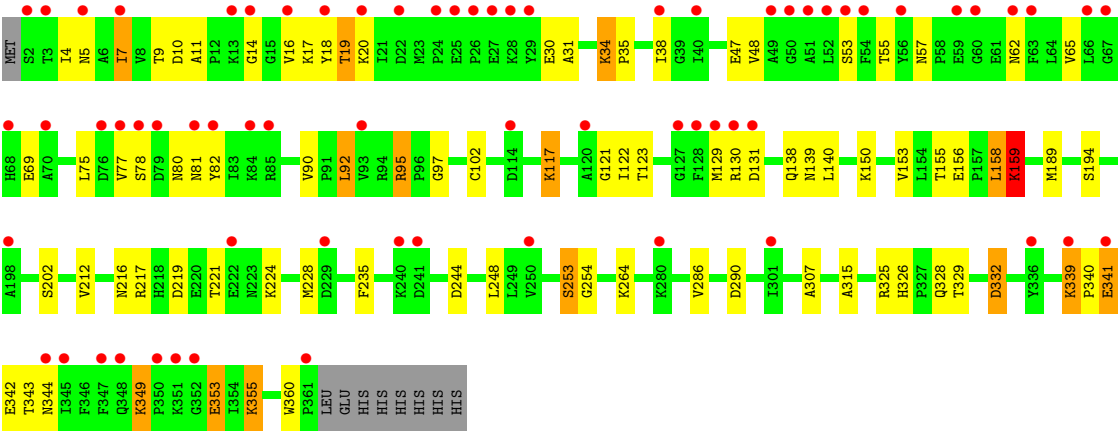


- Molecule 1: Glucose 1-dehydrogenase



- Molecule 1: Glucose 1-dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.91Å 92.33Å 120.47Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	28.01 – 2.33 28.00 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.5 (28.01-2.33) 98.6 (28.00-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.191 , 0.244 0.201 , 0.247	Depositor DCC
R_{free} test set	3752 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.3	EDS
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 74890 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11772	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: DN4, ZN, BGC

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	0.88	0/2887	0.88	1/3904 (0.0%)
1	B	0.92	1/2887 (0.0%)	0.93	3/3904 (0.1%)
1	C	0.83	2/2887 (0.1%)	0.87	5/3904 (0.1%)
1	D	0.79	0/2887	0.86	1/3904 (0.0%)
All	All	0.85	3/11548 (0.0%)	0.88	10/15616 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLU	CD-OE2	-5.44	1.19	1.25
1	C	350	PRO	N-CD	5.36	1.55	1.47
1	C	96	PRO	N-CD	5.11	1.55	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	87	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	306	ASP	CB-CG-OD1	5.46	123.22	118.30
1	C	95	ARG	C-N-CD	5.35	139.63	128.40
1	C	349	LYS	C-N-CD	5.18	139.28	128.40
1	C	148	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	208	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	87	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	D	159	LYS	CA-CB-CG	5.02	124.44	113.40
1	B	217	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	2827	0	2808	33	0
1	B	2827	0	2807	15	0
1	C	2827	0	2807	27	0
1	D	2827	0	2807	54	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	48	0	24	1	0
3	B	48	0	24	1	0
3	C	48	0	24	1	0
3	D	48	0	24	1	0
4	A	12	0	10	1	0
4	B	12	0	12	1	0
4	C	12	0	12	2	0
4	D	12	0	12	1	0
5	A	60	0	0	0	0
5	B	61	0	0	0	0
5	C	51	0	0	0	0
5	D	44	0	0	0	0
All	All	11772	0	11371	130	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 6.

All (130) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:264:LYS:HE3	1:D:290:ASP:OD1	1.68	0.92
1:D:329:THR:HA	1:D:332:ASP:OD2	1.75	0.87
1:D:19:THR:OG1	1:D:20:LYS:N	2.15	0.80
1:D:55:THR:HG22	1:D:122:ILE:HG23	1.65	0.78
1:A:150:LYS:O	1:A:153:VAL:HG12	1.85	0.76
1:A:99:CYS:SG	1:A:102:CYS:HB2	2.27	0.73
1:D:353:GLU:HG3	1:D:353:GLU:O	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:CYS:HB3	1:A:69:GLU:OE2	1.90	0.71
1:D:264:LYS:CE	1:D:290:ASP:OD1	2.40	0.68
1:B:75:LEU:O	1:B:85:ARG:HG3	1.94	0.67
3:A:1003:DN4:C4N	4:A:1004:BGC:H1	2.26	0.65
1:D:69:GLU:OE1	1:D:355:LYS:NZ	2.30	0.65
1:D:156:GLU:O	1:D:159:LYS:HD2	1.97	0.64
1:D:17:LYS:HG3	1:D:19:THR:HG22	1.79	0.63
1:D:92:LEU:HD22	1:D:139:ASN:HA	1.80	0.62
1:D:11:ALA:O	1:D:57:ASN:ND2	2.33	0.60
1:D:7:ILE:HG23	1:D:129:MET:HB3	1.84	0.60
1:A:268:ASN:ND2	1:A:297:ARG:HG2	2.16	0.60
1:D:19:THR:OG1	1:D:20:LYS:O	2.21	0.58
1:C:34:LYS:HE3	1:C:75:LEU:HD21	1.85	0.58
1:D:349:LYS:HB2	1:D:353:GLU:HG2	1.87	0.57
1:D:221:THR:O	1:D:224:LYS:N	2.38	0.57
1:A:303:GLY:O	1:C:174:ARG:NH2	2.23	0.57
1:D:35:PRO:HB2	1:D:38:ILE:HD11	1.87	0.56
1:A:156:GLU:C	1:A:156:GLU:OE2	2.44	0.56
1:A:3:THR:HG23	1:A:22:ASP:OD1	2.05	0.56
1:A:224:LYS:HA	1:A:227:MET:HE3	1.89	0.54
1:C:36:VAL:HG12	1:C:37:TYR:CD2	2.43	0.54
1:D:47:GLU:OE1	1:D:121:GLY:O	2.26	0.54
1:A:159:LYS:HD3	1:A:307:ALA:HB3	1.88	0.54
3:D:1003:DN4:C4N	4:D:1004:BGC:H1	2.38	0.53
1:C:34:LYS:CE	1:C:75:LEU:HD21	2.39	0.53
1:D:4:ILE:O	1:D:20:LYS:HA	2.09	0.52
1:D:16:VAL:HG22	1:D:48:VAL:HG22	1.92	0.52
1:C:81:ASN:N	1:C:81:ASN:OD1	2.43	0.52
1:B:159:LYS:HD2	1:B:307:ALA:HB3	1.91	0.52
1:D:5:ASN:N	1:D:131:ASP:OD2	2.36	0.51
1:A:227:MET:CE	1:A:354:ILE:HD11	2.40	0.51
1:B:159:LYS:CD	1:B:307:ALA:HB3	2.40	0.51
1:D:65:VAL:HG21	1:D:130:ARG:HD3	1.93	0.51
1:D:325:ARG:HG2	1:D:326:HIS:CD2	2.45	0.50
3:B:1003:DN4:C4N	4:B:1004:BGC:H1	2.41	0.50
1:D:339:LYS:O	1:D:342:GLU:N	2.43	0.50
1:B:99:CYS:O	1:B:103:ARG:HD3	2.12	0.50
1:D:30:GLU:O	1:D:77:VAL:HG23	2.12	0.50
1:D:122:ILE:HG22	1:D:123:THR:HG23	1.94	0.49
1:D:18:TYR:CE2	1:D:341:GLU:HG3	2.47	0.49
1:C:284:TYR:CD1	1:C:285:PRO:HD2	2.48	0.49
1:D:55:THR:HG22	1:D:122:ILE:CG2	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:224:LYS:HA	1:A:227:MET:CE	2.42	0.49
1:A:227:MET:HE1	1:A:354:ILE:HD11	1.94	0.49
1:C:159:LYS:HD3	1:C:307:ALA:HB3	1.94	0.49
1:D:31:ALA:HB2	1:D:77:VAL:HG23	1.95	0.48
1:D:328:GLN:O	1:D:332:ASP:OD2	2.32	0.48
1:D:18:TYR:CZ	1:D:340:PRO:HB2	2.49	0.48
1:C:75:LEU:O	1:C:85:ARG:HG2	2.14	0.48
1:D:90:VAL:HG21	1:D:155:THR:HB	1.96	0.48
1:D:158:LEU:HB3	1:D:315:ALA:HB1	1.96	0.47
3:C:1003:DN4:C4N	4:C:1004:BGC:H1	2.44	0.47
1:C:156:GLU:O	1:C:159:LYS:HG3	2.14	0.47
1:C:349:LYS:HE2	1:C:353:GLU:OE1	2.15	0.47
1:D:150:LYS:O	1:D:153:VAL:HG12	2.14	0.47
1:A:7:ILE:HG22	1:A:66:LEU:HD12	1.95	0.47
1:C:306:ASP:OD2	4:C:1004:BGC:O4	2.22	0.47
1:D:228:MET:SD	1:D:235:PHE:HB2	2.54	0.47
1:C:4:ILE:HG21	1:C:132:VAL:HG12	1.96	0.46
1:D:117:LYS:HD2	1:D:117:LYS:O	2.16	0.46
1:D:202:SER:HA	1:D:212:VAL:HG11	1.96	0.46
1:D:18:TYR:HE2	1:D:341:GLU:HG3	1.79	0.46
1:A:223:ASN:C	1:A:227:MET:HE2	2.36	0.46
1:C:216:ASN:OD1	1:C:217:ARG:NH2	2.48	0.46
1:C:34:LYS:HD2	1:C:75:LEU:HD21	1.98	0.46
1:D:18:TYR:CE2	1:D:340:PRO:HB2	2.51	0.46
1:B:223:ASN:H	1:B:223:ASN:HD22	1.62	0.46
1:B:328:GLN:O	1:B:332:ASP:OD2	2.33	0.46
1:C:159:LYS:HE2	1:C:312:TYR:CZ	2.51	0.45
1:D:159:LYS:HG2	1:D:307:ALA:HB3	1.98	0.45
1:D:253:SER:OG	1:D:254:GLY:N	2.50	0.45
1:A:29:TYR:OH	1:A:76:ASP:OD2	2.24	0.45
1:C:336:TYR:CE1	1:C:337:GLU:O	2.70	0.45
1:A:25:GLU:O	1:A:25:GLU:HG3	2.17	0.44
1:A:292:ASP:OD1	1:C:277:PHE:CD1	2.69	0.44
1:A:58:PRO:HG2	1:A:126:HIS:CE1	2.53	0.44
1:A:339:LYS:HD3	1:A:341:GLU:OE2	2.17	0.44
1:D:9:THR:OG1	1:D:14:GLY:HA2	2.18	0.44
1:D:325:ARG:CG	1:D:326:HIS:CD2	3.01	0.44
1:B:283:GLY:HA2	1:D:286:VAL:O	2.18	0.44
1:D:329:THR:CA	1:D:332:ASP:OD2	2.57	0.44
1:C:159:LYS:HE2	1:C:312:TYR:OH	2.18	0.44
1:C:85:ARG:HE	1:C:85:ARG:HB2	1.63	0.43
1:D:95:ARG:HH11	1:D:95:ARG:HG2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:ASN:O	1:A:227:MET:HE2	2.18	0.43
1:D:34:LYS:HG2	1:D:75:LEU:HD11	2.01	0.43
1:C:228:MET:SD	1:C:235:PHE:HB2	2.58	0.43
1:C:4:ILE:HD13	1:C:132:VAL:CG1	2.48	0.43
1:C:75:LEU:O	1:C:85:ARG:CG	2.66	0.43
1:D:97:GLY:N	1:D:102:CYS:SG	2.89	0.43
1:A:92:LEU:HD22	1:A:139:ASN:HA	2.01	0.43
1:D:10:ASP:OD1	1:D:62:ASN:O	2.36	0.43
1:A:326:HIS:HB3	1:A:329:THR:CG2	2.49	0.43
1:A:35:PRO:HB2	1:A:38:ILE:HD11	2.00	0.43
1:C:197:GLU:OE1	1:C:197:GLU:HA	2.18	0.43
1:A:189:MET:HA	1:A:248:LEU:O	2.19	0.42
1:A:326:HIS:HB3	1:A:329:THR:HG22	2.01	0.42
1:A:77:VAL:O	1:A:77:VAL:HG13	2.18	0.42
1:A:240:LYS:C	1:A:241:ASP:OD1	2.58	0.42
1:C:92:LEU:O	1:C:95:ARG:NH2	2.33	0.42
1:C:25:GLU:HG2	1:C:26:PRO:O	2.19	0.42
1:A:215:VAL:HA	1:A:236:SER:O	2.19	0.42
1:B:17:LYS:HG2	1:B:19:THR:HB	2.01	0.42
1:A:201:TYR:OH	1:A:275:PHE:CD1	2.66	0.42
1:B:159:LYS:HD3	1:B:312:TYR:CE1	2.54	0.42
1:C:122:ILE:HG22	1:C:123:THR:HG23	2.02	0.42
1:D:81:ASN:HD22	1:D:81:ASN:N	2.17	0.42
1:B:75:LEU:HA	1:B:75:LEU:HD23	1.87	0.42
1:B:23:MET:CE	1:B:23:MET:HA	2.50	0.41
1:D:216:ASN:OD1	1:D:217:ARG:NH1	2.52	0.41
1:A:153:VAL:HG22	1:A:153:VAL:O	2.21	0.41
1:D:80:ASN:OD1	1:D:82:TYR:N	2.37	0.41
1:D:35:PRO:HG2	1:D:360:TRP:CG	2.56	0.41
1:D:189:MET:HA	1:D:248:LEU:O	2.21	0.41
1:A:132:VAL:C	1:A:133:ILE:HG13	2.40	0.41
1:A:156:GLU:O	1:A:159:LYS:HE3	2.21	0.40
1:B:77:VAL:HG13	1:B:77:VAL:O	2.22	0.40
1:B:156:GLU:O	1:B:159:LYS:HE3	2.21	0.40
1:B:340:PRO:CG	1:B:361:PRO:HD3	2.51	0.40
1:A:215:VAL:HG11	1:A:243:PRO:HG2	2.02	0.40
1:B:237:ASN:ND2	1:B:240:LYS:HE3	2.37	0.40
1:D:9:THR:OG1	1:D:10:ASP:N	2.54	0.40
1:C:151:ILE:HD12	1:C:330:ILE:HG22	2.04	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	358/369 (97%)	344 (96%)	14 (4%)	0	100	100
1	B	358/369 (97%)	348 (97%)	10 (3%)	0	100	100
1	C	358/369 (97%)	338 (94%)	20 (6%)	0	100	100
1	D	358/369 (97%)	342 (96%)	16 (4%)	0	100	100
All	All	1432/1476 (97%)	1372 (96%)	60 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	313/322 (97%)	291 (93%)	22 (7%)	21	23
1	B	313/322 (97%)	297 (95%)	16 (5%)	33	41
1	C	313/322 (97%)	290 (93%)	23 (7%)	20	21
1	D	313/322 (97%)	289 (92%)	24 (8%)	18	19
All	All	1252/1288 (97%)	1167 (93%)	85 (7%)	22	25

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	52	LEU
1	A	59	GLU
1	A	92	LEU
1	A	117	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	VAL
1	A	148	LEU
1	A	159	LYS
1	A	163	LYS
1	A	217	ARG
1	A	225	MET
1	A	241	ASP
1	A	256	PRO
1	A	292	ASP
1	A	304	SER
1	A	306	ASP
1	A	320	SER
1	A	329	THR
1	A	339	LYS
1	A	341	GLU
1	A	344	ASN
1	A	348	GLN
1	B	13	LYS
1	B	23	MET
1	B	92	LEU
1	B	117	LYS
1	B	148	LEU
1	B	150	LYS
1	B	159	LYS
1	B	163	LYS
1	B	178	GLN
1	B	222	GLU
1	B	223	ASN
1	B	229	ASP
1	B	257	SER
1	B	289	GLU
1	B	344	ASN
1	B	361	PRO
1	C	29	TYR
1	C	32	LYS
1	C	34	LYS
1	C	79	ASP
1	C	81	ASN
1	C	85	ARG
1	C	92	LEU
1	C	95	ARG
1	C	117	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	140	LEU
1	C	148	LEU
1	C	150	LYS
1	C	159	LYS
1	C	163	LYS
1	C	194	SER
1	C	225	MET
1	C	229	ASP
1	C	248	LEU
1	C	249	LEU
1	C	257	SER
1	C	264	LYS
1	C	339	LYS
1	C	344	ASN
1	D	7	ILE
1	D	19	THR
1	D	34	LYS
1	D	53	SER
1	D	78	SER
1	D	92	LEU
1	D	95	ARG
1	D	117	LYS
1	D	138	GLN
1	D	140	LEU
1	D	158	LEU
1	D	159	LYS
1	D	194	SER
1	D	219	ASP
1	D	244	ASP
1	D	253	SER
1	D	332	ASP
1	D	339	LYS
1	D	341	GLU
1	D	343	THR
1	D	344	ASN
1	D	349	LYS
1	D	353	GLU
1	D	355	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	118	HIS
1	A	268	ASN
1	A	269	ASN
1	A	324	HIS
1	A	344	ASN
1	A	348	GLN
1	B	118	HIS
1	B	144	ASN
1	B	223	ASN
1	B	269	ASN
1	C	68	HIS
1	C	118	HIS
1	C	138	GLN
1	C	267	ASN
1	C	268	ASN
1	C	269	ASN
1	C	321	ASN
1	C	324	HIS
1	D	5	ASN
1	D	81	ASN
1	D	268	ASN
1	D	321	ASN
1	D	324	HIS
1	D	326	HIS
1	D	348	GLN

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 ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
3	DN4	A	1003	-	52,52,52	2.01	13 (25%)	80,80,80	1.82	14 (17%)
4	BGC	A	1004	-	12,12,12	1.99	4 (33%)	17,17,17	1.57	4 (23%)
3	DN4	B	1003	-	52,52,52	1.91	12 (23%)	80,80,80	3.58	21 (26%)
4	BGC	B	1004	-	12,12,12	1.69	3 (25%)	17,17,17	1.41	2 (11%)
3	DN4	C	1003	-	52,52,52	1.89	15 (28%)	80,80,80	2.45	17 (21%)
4	BGC	C	1004	-	12,12,12	0.84	0	17,17,17	0.66	0
3	DN4	D	1003	-	52,52,52	1.95	14 (26%)	80,80,80	2.41	24 (30%)
4	BGC	D	1004	-	12,12,12	1.25	1 (8%)	17,17,17	1.70	5 (29%)

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
3	DN4	A	1003	-	-	0/35/67/67	0/5/5/5
4	BGC	A	1004	-	-	0/2/22/22	0/1/1/1
3	DN4	B	1003	-	-	1/35/67/67	0/5/5/5
4	BGC	B	1004	-	-	0/2/22/22	0/1/1/1
3	DN4	C	1003	-	-	0/35/67/67	0/5/5/5
4	BGC	C	1004	-	-	0/2/22/22	0/1/1/1
3	DN4	D	1003	-	-	0/35/67/67	0/5/5/5
4	BGC	D	1004	-	-	0/2/22/22	0/1/1/1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1003	DN4	C2A-N3A	5.98	1.42	1.32
3	C	1003	DN4	PN-O3	5.86	1.72	1.60
3	A	1003	DN4	PN-O3	5.56	1.71	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1003	DN4	C2N-N1N	5.19	1.42	1.35
3	B	1003	DN4	O4B-C1B	5.10	1.47	1.41
3	B	1003	DN4	O4D-C1D	4.73	1.47	1.41
3	A	1003	DN4	C2N-N1N	4.26	1.40	1.35
3	A	1003	DN4	C3N-C7N	-4.20	1.40	1.49
3	B	1003	DN4	C2A-N3A	3.99	1.39	1.32
4	A	1004	BGC	C1-C2	-3.88	1.45	1.52
3	A	1003	DN4	C2A-N3A	3.84	1.38	1.32
3	A	1003	DN4	C2D-C1D	-3.83	1.47	1.53
4	A	1004	BGC	O2-C2	-3.83	1.33	1.43
3	B	1003	DN4	O7N-C7N	3.72	1.34	1.23
3	B	1003	DN4	PN-O3	3.67	1.68	1.60
3	C	1003	DN4	PA-O3	3.63	1.66	1.59
3	C	1003	DN4	C2N-N1N	3.61	1.39	1.35
3	B	1003	DN4	C4A-N9A	-3.59	1.32	1.37
3	B	1003	DN4	C2B-C1B	-3.58	1.46	1.52
3	A	1003	DN4	PA-O3	3.56	1.66	1.59
3	C	1003	DN4	C5A-C4A	-3.53	1.32	1.40
3	B	1003	DN4	C2N-N1N	3.50	1.39	1.35
4	B	1004	BGC	C1-C2	-3.49	1.46	1.52
3	A	1003	DN4	C4A-N9A	-3.47	1.32	1.37
3	C	1003	DN4	C4A-N9A	-3.45	1.32	1.37
3	D	1003	DN4	C8A-N9A	-3.44	1.31	1.36
3	A	1003	DN4	O4D-C1D	3.38	1.45	1.41
3	D	1003	DN4	PN-O3	3.36	1.67	1.60
3	C	1003	DN4	C2D-C1D	-3.31	1.48	1.53
3	A	1003	DN4	C2A-N1A	3.26	1.40	1.33
3	D	1003	DN4	P2B-O2B	3.25	1.69	1.59
3	D	1003	DN4	PA-O3	3.14	1.65	1.59
3	C	1003	DN4	C2A-N3A	3.09	1.37	1.32
3	C	1003	DN4	O7N-C7N	3.03	1.32	1.23
3	D	1003	DN4	O4D-C1D	2.99	1.45	1.41
3	A	1003	DN4	P2B-O3X	2.99	1.65	1.54
3	D	1003	DN4	C2A-N1A	2.90	1.39	1.33
3	B	1003	DN4	C5A-C4A	-2.89	1.34	1.40
4	D	1004	BGC	O5-C1	2.88	1.48	1.43
3	B	1003	DN4	P2B-O2B	2.77	1.68	1.59
3	C	1003	DN4	C3N-C7N	-2.73	1.43	1.49
3	C	1003	DN4	P2B-O2B	2.73	1.68	1.59
3	D	1003	DN4	O7N-C7N	2.57	1.30	1.23
3	C	1003	DN4	P2B-O2X	2.55	1.63	1.54
3	A	1003	DN4	C5A-C4A	-2.50	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	DN4	P2B-O2B	2.49	1.67	1.59
3	C	1003	DN4	O4B-C1B	2.47	1.44	1.41
3	D	1003	DN4	C3N-C7N	-2.42	1.44	1.49
3	D	1003	DN4	C5A-C4A	-2.40	1.35	1.40
3	C	1003	DN4	C2A-N1A	2.35	1.38	1.33
3	D	1003	DN4	C2D-C1D	-2.32	1.50	1.53
3	B	1003	DN4	C3N-C7N	-2.31	1.44	1.49
4	B	1004	BGC	O5-C5	-2.29	1.38	1.44
3	C	1003	DN4	C6N-N1N	2.29	1.41	1.35
3	A	1003	DN4	O7N-C7N	2.28	1.30	1.23
3	C	1003	DN4	PN-O5D	2.25	1.67	1.59
4	A	1004	BGC	C4-C5	-2.22	1.48	1.53
3	D	1003	DN4	PN-O5D	2.14	1.66	1.59
4	B	1004	BGC	O2-C2	-2.13	1.37	1.43
4	A	1004	BGC	O5-C5	-2.13	1.39	1.44
3	D	1003	DN4	C4A-N9A	-2.08	1.34	1.37
3	B	1003	DN4	C8A-N9A	-2.04	1.33	1.36

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	DN4	O4D-C1D-N1N	-21.56	84.45	108.13
3	B	1003	DN4	N3A-C2A-N1A	-14.94	115.74	128.89
3	C	1003	DN4	N3A-C2A-N1A	-13.39	117.11	128.89
3	D	1003	DN4	O4D-C1D-N1N	-10.88	96.18	108.13
3	D	1003	DN4	N3A-C2A-N1A	-9.97	120.12	128.89
3	A	1003	DN4	N3A-C2A-N1A	-8.88	121.08	128.89
3	B	1003	DN4	C1B-N9A-C4A	-8.71	111.58	126.64
3	C	1003	DN4	C1B-N9A-C4A	-7.00	114.54	126.64
3	B	1003	DN4	C8A-N9A-C1B	6.97	139.27	126.15
3	D	1003	DN4	C5A-C4A-N3A	-5.54	120.58	125.98
3	C	1003	DN4	C8A-N9A-C1B	5.51	136.53	126.15
3	C	1003	DN4	O4D-C1D-N1N	-5.03	102.61	108.13
3	D	1003	DN4	C1B-N9A-C4A	-4.70	118.51	126.64
3	C	1003	DN4	C4D-O4D-C1D	-4.63	104.63	109.72
3	A	1003	DN4	C4B-O4B-C1B	-4.62	104.64	109.72
3	A	1003	DN4	C1B-N9A-C4A	-4.44	118.97	126.64
3	C	1003	DN4	C5A-C4A-N3A	-4.39	121.70	125.98
3	B	1003	DN4	C4D-O4D-C1D	-4.36	104.92	109.72
3	D	1003	DN4	C4A-C5A-N7A	-4.32	105.24	109.41
3	D	1003	DN4	C4B-O4B-C1B	-4.30	105.00	109.72
3	A	1003	DN4	C4D-O4D-C1D	-4.28	105.02	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	DN4	O4D-C1D-C2D	-4.24	100.52	106.69
3	B	1003	DN4	C2D-C1D-N1N	4.09	121.67	113.48
3	C	1003	DN4	C4B-O4B-C1B	-4.05	105.27	109.72
3	A	1003	DN4	C5A-C4A-N3A	-3.93	122.15	125.98
4	D	1004	BGC	O5-C5-C6	3.84	115.90	106.34
3	B	1003	DN4	C5A-C4A-N3A	-3.71	122.36	125.98
3	D	1003	DN4	C8A-N9A-C1B	3.52	132.77	126.15
3	B	1003	DN4	C4B-O4B-C1B	-3.49	105.88	109.72
4	B	1004	BGC	O5-C5-C6	-3.48	97.67	106.34
3	C	1003	DN4	O2X-P2B-O2B	-3.47	97.10	107.09
4	A	1004	BGC	O5-C5-C6	-3.47	97.71	106.34
3	A	1003	DN4	C8A-N9A-C1B	3.24	132.25	126.15
3	D	1003	DN4	C6A-C5A-C4A	3.16	121.10	117.55
3	B	1003	DN4	O2X-P2B-O2B	-3.13	98.08	107.09
4	A	1004	BGC	O1-C1-O5	-3.10	101.71	110.29
3	B	1003	DN4	PN-O3-PA	-3.01	121.08	133.17
3	D	1003	DN4	O2X-P2B-O2B	-2.95	98.61	107.09
4	B	1004	BGC	C1-O5-C5	2.87	118.77	113.43
3	A	1003	DN4	C6A-C5A-C4A	2.83	120.73	117.55
3	B	1003	DN4	C2N-C3N-C7N	2.80	124.81	119.78
3	D	1003	DN4	O3X-P2B-O1X	2.72	119.27	110.36
3	B	1003	DN4	C2N-C3N-C4N	-2.70	115.29	118.31
3	D	1003	DN4	N3A-C4A-N9A	2.68	129.99	125.39
4	D	1004	BGC	O5-C1-C2	2.67	114.13	109.80
3	B	1003	DN4	C8A-N9A-C4A	2.64	109.10	106.96
3	D	1003	DN4	C2D-C1D-N1N	2.64	118.75	113.48
3	B	1003	DN4	C2A-N3A-C4A	2.63	120.85	113.27
3	A	1003	DN4	O2X-P2B-O2B	-2.59	99.65	107.09
3	C	1003	DN4	N7A-C8A-N9A	-2.56	106.40	112.20
3	D	1003	DN4	C2N-C3N-C4N	-2.55	115.45	118.31
3	B	1003	DN4	C3D-C2D-C1D	-2.54	96.94	100.92
3	B	1003	DN4	O2B-P2B-O1X	2.52	114.03	106.80
3	C	1003	DN4	N3A-C4A-N9A	2.51	129.71	125.39
3	A	1003	DN4	N3A-C4A-N9A	2.50	129.68	125.39
3	C	1003	DN4	C2A-N3A-C4A	2.49	120.43	113.27
4	A	1004	BGC	C1-C2-C3	-2.44	106.87	110.48
4	D	1004	BGC	C4-C3-C2	-2.43	106.33	110.80
3	B	1003	DN4	O2X-P2B-O1X	2.39	118.19	110.36
3	D	1003	DN4	N7A-C8A-N9A	-2.39	106.78	112.20
3	C	1003	DN4	C8A-N9A-C4A	2.38	108.89	106.96
3	A	1003	DN4	O3-PA-O5B	2.38	109.21	102.91
3	B	1003	DN4	N3A-C4A-N9A	2.37	129.46	125.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	DN4	C3B-C2B-C1B	-2.35	98.18	102.70
3	B	1003	DN4	C5N-C4N-C3N	2.34	123.26	120.34
4	D	1004	BGC	C3-C4-C5	-2.32	106.01	110.17
3	C	1003	DN4	C3D-C2D-C1D	-2.29	97.32	100.92
4	D	1004	BGC	O5-C5-C4	-2.26	105.52	109.73
3	B	1003	DN4	C5N-C6N-N1N	-2.25	116.71	120.49
3	A	1003	DN4	C8A-N9A-C4A	2.23	108.77	106.96
3	C	1003	DN4	C2N-N1N-C1D	-2.21	113.85	119.33
3	C	1003	DN4	O4B-C1B-C2B	-2.17	102.63	106.60
3	B	1003	DN4	O3X-P2B-O2X	-2.18	99.22	107.38
3	D	1003	DN4	C8A-N9A-C4A	2.16	108.72	106.96
3	D	1003	DN4	O4D-C4D-C5D	2.13	116.92	109.37
3	D	1003	DN4	C3B-C2B-C1B	-2.12	98.62	102.70
3	D	1003	DN4	C4D-O4D-C1D	-2.07	107.44	109.72
3	D	1003	DN4	C5N-C4N-C3N	2.08	122.93	120.34
3	D	1003	DN4	O2B-P2B-O1X	2.06	112.73	106.80
3	C	1003	DN4	C6N-N1N-C1D	2.06	124.43	119.33
3	A	1003	DN4	O2A-PA-O1A	2.04	123.41	112.14
4	A	1004	BGC	C3-C4-C5	-2.03	106.52	110.17
3	D	1003	DN4	O4B-C1B-C2B	-2.03	102.90	106.60
3	A	1003	DN4	O2D-C2D-C1D	-2.03	105.07	111.49
3	D	1003	DN4	C8A-N7A-C5A	2.01	109.83	103.58
3	D	1003	DN4	O3D-C3D-C4D	-2.01	105.16	111.07
3	D	1003	DN4	O4B-C1B-N9A	-2.00	103.74	108.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	DN4	C2D-C1D-N1N-C2N

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	360/369 (97%)	0.44	33 (9%) 9 15	24, 45, 74, 95	0
1	B	360/369 (97%)	0.14	13 (3%) 41 52	23, 38, 68, 96	0
1	C	360/369 (97%)	0.47	39 (10%) 6 10	25, 47, 77, 114	0
1	D	360/369 (97%)	0.89	68 (18%) 2 3	25, 55, 95, 126	0
All	All	1440/1476 (97%)	0.48	153 (10%) 7 11	23, 46, 82, 126	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	PRO	7.3
1	D	352	GLY	7.2
1	D	60	GLY	7.1
1	D	351	LYS	7.0
1	D	79	ASP	6.8
1	D	28	LYS	6.4
1	B	28	LYS	5.6
1	C	27	GLU	5.5
1	D	27	GLU	5.2
1	C	60	GLY	5.0
1	D	29	TYR	4.9
1	D	350	PRO	4.9
1	D	85	ARG	4.8
1	A	352	GLY	4.6
1	D	50	GLY	4.5
1	D	82	TYR	4.3
1	A	53	SER	4.3
1	C	82	TYR	4.3
1	B	50	GLY	4.2
1	D	62	ASN	4.2
1	D	51	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	25	GLU	4.1
1	A	60	GLY	4.1
1	C	240	LYS	4.0
1	B	280	LYS	4.0
1	D	24	PRO	4.0
1	D	38	ILE	4.0
1	D	66	LEU	3.9
1	A	351	LYS	3.9
1	D	2	SER	3.8
1	C	280	LYS	3.8
1	D	128	PHE	3.7
1	D	16	VAL	3.7
1	D	336	TYR	3.6
1	A	13	LYS	3.6
1	D	222	GLU	3.5
1	C	26	PRO	3.5
1	D	240	LYS	3.5
1	C	79	ASP	3.5
1	A	274	LEU	3.5
1	D	84	LYS	3.5
1	D	76	ASP	3.5
1	D	347	PHE	3.4
1	C	351	LYS	3.4
1	C	348	GLN	3.4
1	A	59	GLU	3.4
1	D	348	GLN	3.4
1	A	79	ASP	3.3
1	C	85	ARG	3.3
1	D	129	MET	3.3
1	C	272	VAL	3.3
1	D	127	GLY	3.3
1	C	223	ASN	3.2
1	D	5	ASN	3.2
1	A	240	LYS	3.2
1	D	3	THR	3.2
1	A	348	GLN	3.2
1	D	18	TYR	3.1
1	C	28	LYS	3.1
1	A	40	ILE	3.1
1	A	223	ASN	3.1
1	A	222	GLU	3.1
1	B	82	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	53	SER	3.0
1	D	59	GLU	3.0
1	A	81	ASN	3.0
1	D	81	ASN	3.0
1	A	85	ARG	3.0
1	D	280	LYS	2.9
1	D	241	ASP	2.9
1	D	344	ASN	2.9
1	D	54	PHE	2.9
1	D	68	HIS	2.9
1	D	22	ASP	2.9
1	B	81	ASN	2.9
1	C	241	ASP	2.9
1	A	49	ALA	2.8
1	C	77	VAL	2.8
1	B	13	LYS	2.8
1	C	2	SER	2.8
1	A	62	ASN	2.8
1	D	20	LYS	2.8
1	B	351	LYS	2.8
1	A	241	ASP	2.8
1	C	22	ASP	2.8
1	A	280	LYS	2.7
1	D	250	VAL	2.7
1	A	347	PHE	2.7
1	D	70	ALA	2.7
1	D	56	TYR	2.6
1	A	54	PHE	2.6
1	C	84	LYS	2.6
1	A	239	LEU	2.6
1	A	20	LYS	2.6
1	D	14	GLY	2.6
1	D	361	PRO	2.6
1	C	281	ALA	2.6
1	D	120	ALA	2.6
1	D	67	GLY	2.5
1	A	82	TYR	2.5
1	C	81	ASN	2.5
1	B	53	SER	2.5
1	C	226	LYS	2.4
1	A	68	HIS	2.4
1	C	80	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	24	PRO	2.4
1	B	274	LEU	2.3
1	D	229	ASP	2.3
1	A	250	VAL	2.3
1	C	328	GLN	2.3
1	D	93	VAL	2.3
1	B	26	PRO	2.3
1	C	350	PRO	2.3
1	C	192	ILE	2.3
1	C	301	ILE	2.3
1	D	341	GLU	2.3
1	A	219	ASP	2.3
1	D	345	ILE	2.3
1	B	79	ASP	2.3
1	D	131	ASP	2.3
1	D	52	LEU	2.3
1	D	78	SER	2.2
1	C	352	GLY	2.2
1	C	93	VAL	2.2
1	D	77	VAL	2.2
1	B	348	GLN	2.2
1	D	301	ILE	2.2
1	C	250	VAL	2.2
1	D	339	LYS	2.2
1	A	127	GLY	2.2
1	A	273	ILE	2.2
1	D	49	ALA	2.2
1	C	249	LEU	2.2
1	D	7	ILE	2.1
1	D	13	LYS	2.1
1	D	40	ILE	2.1
1	D	63	PHE	2.1
1	C	154	LEU	2.1
1	A	70	ALA	2.1
1	A	272	VAL	2.1
1	B	250	VAL	2.1
1	C	68	HIS	2.1
1	D	130	ARG	2.1
1	C	29	TYR	2.1
1	C	40	ILE	2.1
1	A	325	ARG	2.1
1	C	157	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	339	LYS	2.0
1	D	114	ASP	2.0
1	C	283	GLY	2.0
1	C	13	LYS	2.0
1	D	198	ALA	2.0
1	A	10	ASP	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
4	BGC	B	1004	12/12	0.21	1.39	51,64,73,73	0
4	BGC	C	1004	12/12	0.20	0.48	61,79,93,93	0
4	BGC	D	1004	12/12	0.18	-0.13	66,77,85,91	0
3	DN4	C	1003	48/48	0.13	-0.30	43,65,95,109	0
2	ZN	D	1002	1/1	0.10	-0.50	34,34,34,34	0
3	DN4	D	1003	48/48	0.14	-0.56	44,68,92,101	0
4	BGC	A	1004	12/12	0.12	-0.70	48,67,88,93	0
2	ZN	A	1001	1/1	0.14	-0.73	71,71,71,71	0
2	ZN	D	1001	1/1	0.16	-0.73	89,89,89,89	0
3	DN4	B	1003	48/48	0.13	-0.76	40,56,77,80	0
2	ZN	C	1001	1/1	0.14	-0.90	71,71,71,71	0
2	ZN	B	1002	1/1	0.07	-0.98	32,32,32,32	0
2	ZN	A	1002	1/1	0.08	-1.00	34,34,34,34	0
3	DN4	A	1003	48/48	0.12	-1.17	38,67,85,95	0
2	ZN	C	1002	1/1	0.06	-1.76	35,35,35,35	0
2	ZN	B	1001	1/1	0.05	-5.07	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.