



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2018 – 11:52 PM EST

PDB ID : 6EJK
Title : Structure of a glycosyltransferase
Authors : Ramirez, A.S.; Boilevin, J.; Mehdipour, A.R.; Hummer, G.; Darbre, T.; Raymond, J.L.; Locher, K.P.
Deposited on : 2017-09-21
Resolution : 3.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

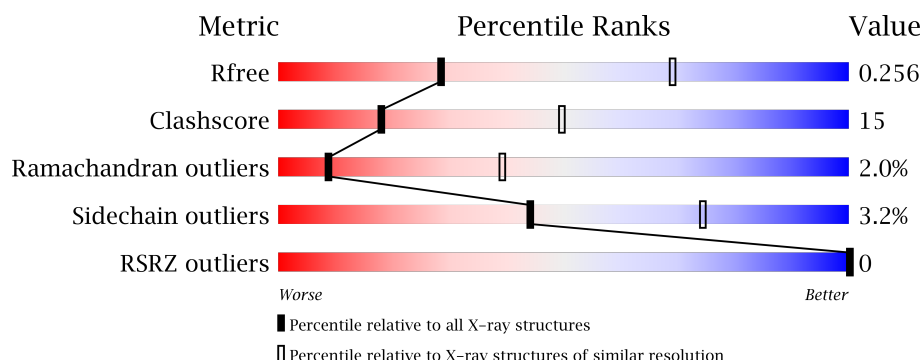
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.30 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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	373	 62% 33% . .
1	B	373	 62% 32% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6012 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 WlaC protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	Se	0	0	0
			2914	1886	486	529	9	4			
1	B	360	Total	C	N	O	S	Se	0	0	0
			2914	1886	486	529	9	4			

There are 32 discrepancies between the modelled and reference sequences:

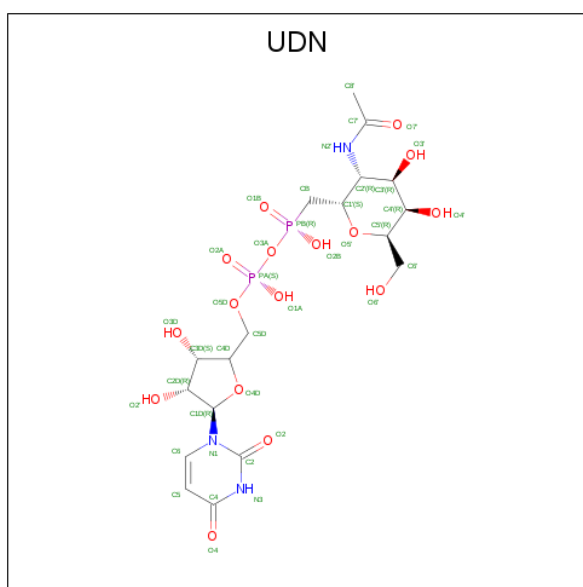
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP O86151
A	2	MSE	-	expression tag	UNP O86151
A	3	MSE	-	expression tag	UNP O86151
A	361	LEU	-	expression tag	UNP O86151
A	362	GLY	-	expression tag	UNP O86151
A	363	SER	-	expression tag	UNP O86151
A	364	HIS	-	expression tag	UNP O86151
A	365	HIS	-	expression tag	UNP O86151
A	366	HIS	-	expression tag	UNP O86151
A	367	HIS	-	expression tag	UNP O86151
A	368	HIS	-	expression tag	UNP O86151
A	369	HIS	-	expression tag	UNP O86151
A	370	HIS	-	expression tag	UNP O86151
A	371	HIS	-	expression tag	UNP O86151
A	372	HIS	-	expression tag	UNP O86151
A	373	HIS	-	expression tag	UNP O86151
B	1	MSE	-	initiating methionine	UNP O86151
B	2	MSE	-	expression tag	UNP O86151
B	3	MSE	-	expression tag	UNP O86151
B	361	LEU	-	expression tag	UNP O86151
B	362	GLY	-	expression tag	UNP O86151
B	363	SER	-	expression tag	UNP O86151
B	364	HIS	-	expression tag	UNP O86151
B	365	HIS	-	expression tag	UNP O86151
B	366	HIS	-	expression tag	UNP O86151

Continued on next page...

Continued from previous page...

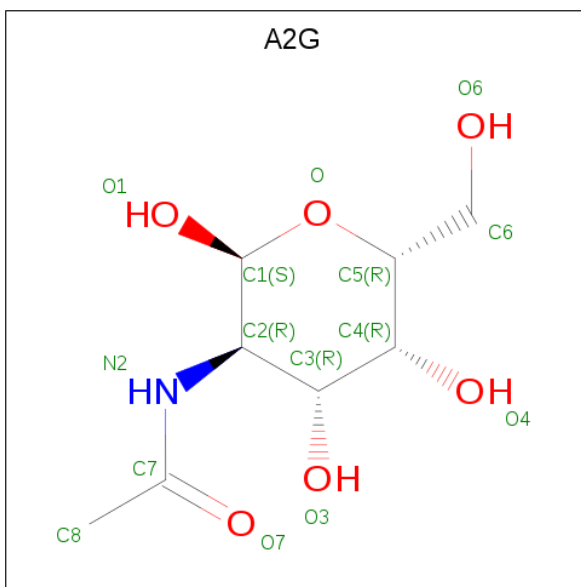
Chain	Residue	Modelled	Actual	Comment	Reference
B	367	HIS	-	expression tag	UNP O86151
B	368	HIS	-	expression tag	UNP O86151
B	369	HIS	-	expression tag	UNP O86151
B	370	HIS	-	expression tag	UNP O86151
B	371	HIS	-	expression tag	UNP O86151
B	372	HIS	-	expression tag	UNP O86151
B	373	HIS	-	expression tag	UNP O86151

- Molecule 2 is Uridine-Diphosphate-Methylene-N-acetyl-galactosamine (three-letter code: UDN) (formula: $C_{18}H_{29}N_3O_{16}P_2$).



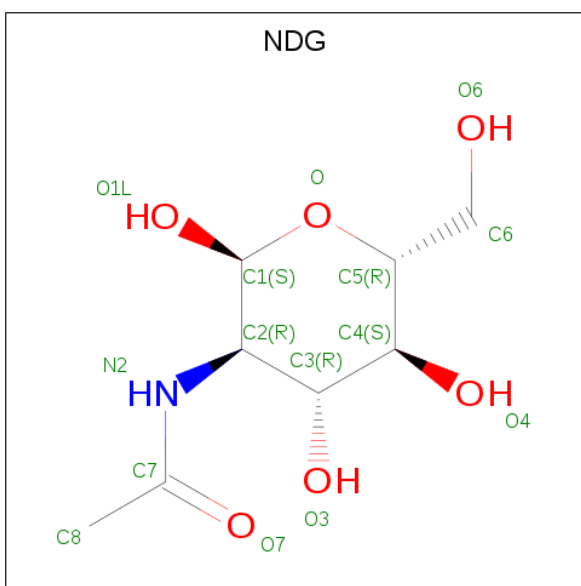
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	18	3	16	2		
2	B	1	Total	C	N	O	P	0	0
			39	18	3	16	2		

- Molecule 3 is N-ACETYL-2-DEOXY-2-AMINO-GALACTOSE (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



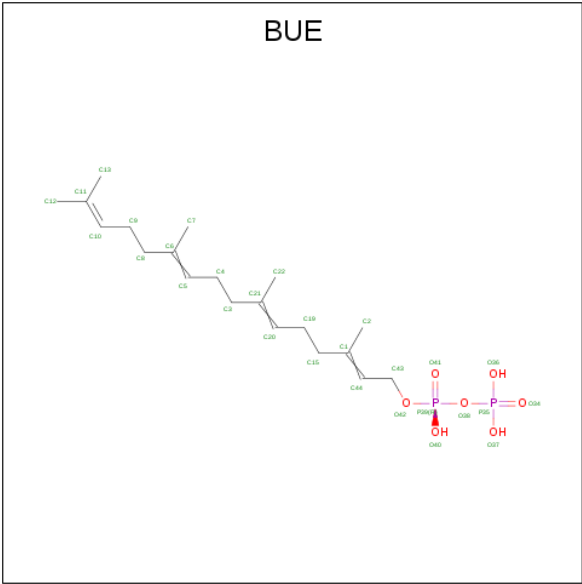
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is NerylNeryl pyrophosphate (three-letter code: BUE) (formula: C₂₀H₃₆O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			11	2	7	2		
5	B	1	Total	C	O	P	0	0
			11	2	7	2		

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

- Chain A:  62% 33%

- Chain B: 62% 32%

Row	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9	Col 10	Col 11	Col 12	Col 13	Col 14	Col 15	Col 16
1	M1	A105	L212	D309	M2	N106	K217	V219	K316	K317	E318	L319	V320	L321	E324	R327
2	K3	N107	V219	K316	K4	L113	F218	V219	L317	E318	L319	V320	L321	E324	R327	M1
3	T5	P112	V219	K316	S6	L113	F218	V219	L317	E318	L319	V320	L321	E324	R327	M2
4	F7	L115	V219	K316	T8	L115	F218	V219	L317	E318	L319	V320	L321	E324	R327	K4
5	I9	S117	V219	K316	I9	S117	F218	V219	L317	E318	L319	V320	L321	E324	R327	T5
6	L12	H118	V219	K316	L12	H118	F218	V219	L317	E318	L319	V320	L321	E324	R327	S6
7	N13	S119	V219	K316	N13	S119	F218	V219	L317	E318	L319	V320	L321	E324	R327	F7
8	S14	M120	V219	K316	S14	M120	F218	V219	L317	E318	L319	V320	L321	E324	R327	I9
9	G15	A121	V219	K316	G15	A121	F218	V219	L317	E318	L319	V320	L321	E324	R327	L12
10	V20	A122	V219	K316	V20	A122	F218	V219	L317	E318	L319	V320	L321	E324	R327	N13
11	L21	A123	V219	K316	L21	A123	F218	V219	L317	E318	L319	V320	L321	E324	R327	S14
12	V22	T128	V219	K316	V22	T128	F218	V219	L317	E318	L319	V320	L321	E324	R327	G15
13	A25	M129	V219	K316	A25	M129	F218	V219	L317	E318	L319	V320	L321	E324	R327	V20
14	M26	F131	V219	K316	M26	F131	F218	V219	L317	E318	L319	V320	L321	E324	R327	L21
15	A27	L132	V219	K316	A27	L132	F218	V219	L317	E318	L319	V320	L321	E324	R327	V22
16	L28	R133	V219	K316	L28	R133	F218	V219	L317	E318	L319	V320	L321	E324	R327	A25
17	C29	R134	V219	K316	C29	R134	F218	V219	L317	E318	L319	V320	L321	E324	R327	M26
18	S35	Y137	V219	K316	S35	Y137	F218	V219	L317	E318	L319	V320	L321	E324	R327	A27
19	I36	S144	V219	K316	I36	S144	F218	V219	L317	E318	L319	V320	L321	E324	R327	L28
20	L37	V145	V219	K316	L37	V145	F218	V219	L317	E318	L319	V320	L321	E324	R327	C29
21	K38	F145	V219	K316	K38	F145	F218	V219	L317	E318	L319	V320	L321	E324	R327	S35
22	F45	D150	V219	K316	F45	D150	F218	V219	L317	E318	L319	V320	L321	E324	R327	I36
23	L48	K151	V219	K316	L48	K151	F218	V219	L317	E318	L319	V320	L321	E324	R327	L37
24	N50	V152	V219	K316	N50	V152	F218	V219	L317	E318	L319	V320	L321	E324	R327	K38
25	E51	F157	V219	K316	E51	F157	F218	V219	L317	E318	L319	V320	L321	E324	R327	F45
26	R61	L164	V219	K316	R61	L164	F218	V219	L317	E318	L319	V320	L321	E324	R327	L48

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.87Å 126.91Å 71.09Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	29.89 – 3.30 29.89 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.89-3.30) 87.1 (29.89-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.254 0.215 , 0.256	Depositor DCC
R_{free} test set	832 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 4.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6012	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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: A2G, UDN, NDG, BUE

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	0.65	1/2965 (0.0%)	0.69	0/3983
1	B	0.61	0/2965	0.68	0/3983
All	All	0.63	1/5930 (0.0%)	0.69	0/7966

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	CYS	CB-SG	-6.47	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2914	0	2992	91	0
1	B	2914	0	2992	84	0
2	A	39	0	0	3	0
2	B	39	0	0	2	0
3	A	28	0	25	6	0
3	B	28	0	25	8	0
4	A	14	0	12	1	0
4	B	14	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	11	0	0	0	0
5	B	11	0	0	0	0
All	All	6012	0	6058	182	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 (182) 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)
3:B:403:A2G:O6	3:B:403:A2G:C6	1.64	1.45
3:A:403:A2G:O6	3:A:403:A2G:C6	1.68	1.40
1:A:280:GLU:HA	1:A:331:VAL:HG11	1.33	1.08
1:B:324:GLU:OE2	1:B:327:ARG:NH1	1.86	1.08
1:B:324:GLU:CD	1:B:327:ARG:HH11	1.65	0.99
1:A:116:SER:HB3	1:A:144:SER:HB3	1.47	0.93
1:B:280:GLU:HA	1:B:331:VAL:HG11	1.48	0.93
1:B:22:VAL:HG13	1:B:48:LEU:HD13	1.56	0.87
3:B:403:A2G:C5	3:B:403:A2G:O6	2.33	0.75
1:A:22:VAL:HG13	1:A:48:LEU:HD13	1.70	0.74
1:B:29:CYS:SG	1:B:51:GLU:HB2	2.27	0.73
1:A:247:VAL:N	2:A:401:UDN:O4	2.20	0.73
1:B:116:SER:HB3	1:B:144:SER:HB3	1.74	0.69
3:A:403:A2G:N2	4:A:404:NDG:O4	2.26	0.69
1:B:191:ARG:NH1	3:B:402:A2G:H2	2.08	0.68
1:B:266:VAL:HG23	1:B:289:TYR:HB3	1.76	0.67
1:A:266:VAL:HG23	1:A:289:TYR:HB3	1.76	0.67
1:A:115:ILE:HD11	1:A:140:CYS:SG	2.35	0.67
1:A:188:PHE:HD2	1:A:220:ILE:HG23	1.61	0.66
1:B:247:VAL:N	2:B:401:UDN:O4	2.27	0.65
3:A:403:A2G:O6	3:A:403:A2G:C5	2.44	0.65
1:A:61:ARG:HH12	1:B:248:GLU:CD	2.00	0.64
1:A:280:GLU:CA	1:A:331:VAL:HG11	2.18	0.63
1:A:85:GLU:HG2	1:A:85:GLU:O	1.99	0.63
1:A:169:HIS:HA	1:A:343:ILE:HD11	1.81	0.62
1:A:309:ASP:HB3	1:A:312:ALA:HB3	1.80	0.62
1:B:309:ASP:HB3	1:B:312:ALA:HB3	1.81	0.62
1:B:121:GLU:OE1	1:B:130:ARG:NH2	2.31	0.61
1:A:342:GLU:CD	1:A:344:SER:OG	2.38	0.61
1:B:133:ARG:O	1:B:137:TYR:HB2	2.00	0.60
1:A:251:LYS:O	1:A:255:GLU:HG3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:OG	1:A:115:ILE:HG22	2.03	0.59
1:B:98:THR:OG1	3:B:403:A2G:H8	2.03	0.58
1:B:200:MSE:HE1	1:B:305:VAL:HG21	1.86	0.58
1:B:26:ASN:OD1	1:B:49:GLU:HB2	2.04	0.58
1:B:298:ASP:HB2	1:B:304:LEU:HD12	1.85	0.57
1:A:61:ARG:NH1	1:B:248:GLU:CD	2.57	0.57
3:A:403:A2G:H15	3:A:403:A2G:C6	2.11	0.57
1:A:64:THR:HG22	1:A:66:TYR:H	1.70	0.57
1:B:301:ASP:HB2	1:B:334:ALA:HB2	1.85	0.56
1:A:196:LYS:NZ	2:A:401:UDN:O2B	2.39	0.56
1:B:251:LYS:O	1:B:255:GLU:HG3	2.06	0.56
1:B:2:MSE:HG3	1:B:3:MSE:N	2.20	0.56
3:B:403:A2G:H15	3:B:403:A2G:C6	2.08	0.56
1:B:61:ARG:O	1:B:67:HIS:HB3	2.06	0.55
1:A:13:ASN:O	1:A:15:GLY:N	2.39	0.55
1:A:50:ASN:O	1:B:61:ARG:NH2	2.39	0.55
1:A:342:GLU:HB3	1:A:345:ASN:ND2	2.22	0.55
1:A:233:LYS:HA	1:A:236:SER:HB3	1.89	0.55
1:B:284:ILE:HG12	1:B:303:LEU:HB2	1.89	0.55
1:A:138:PRO:HB3	1:A:157:PHE:O	2.07	0.54
1:A:292:ALA:HB3	1:A:293:LYS:NZ	2.22	0.54
1:A:280:GLU:HA	1:A:331:VAL:CG1	2.22	0.54
1:A:187:LEU:HD13	1:A:189:ILE:HD11	1.90	0.54
1:A:342:GLU:HG2	1:A:344:SER:OG	2.07	0.53
1:A:223:ASP:OD1	1:A:227:ARG:HD3	2.07	0.53
1:A:181:GLU:OE1	1:A:181:GLU:N	2.41	0.53
1:B:217:LYS:NZ	1:B:217:LYS:HB3	2.23	0.53
1:B:222:GLY:O	1:B:245:GLY:HA2	2.08	0.53
1:B:192:LEU:HD13	1:B:230:LEU:HD12	1.91	0.53
1:B:145:VAL:HG21	1:B:150:ASP:HB3	1.91	0.52
1:A:9:ILE:O	1:A:38:LYS:HA	2.10	0.52
1:A:12:LEU:HD13	1:A:44:SER:HB2	1.91	0.52
1:B:96:ASP:CG	1:B:97:THR:H	2.14	0.52
1:A:22:VAL:HG12	1:A:26:ASN:ND2	2.25	0.52
1:B:6:SER:OG	1:B:35:SER:HB3	2.10	0.51
1:B:316:LYS:O	1:B:319:LEU:HB3	2.10	0.51
1:A:116:SER:HB3	1:A:144:SER:CB	2.30	0.51
1:A:98:THR:OG1	3:A:403:A2G:H8	2.11	0.51
1:B:271:THR:O	1:B:275:GLU:HG3	2.11	0.51
2:B:401:UDN:O6'	2:B:401:UDN:O4'	2.27	0.51
1:B:191:ARG:HH12	3:B:402:A2G:H2	1.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PHE:HB2	1:B:36:ILE:HG12	1.93	0.51
1:B:114:ILE:O	1:B:115:ILE:HG12	2.11	0.50
1:B:233:LYS:HA	1:B:236:SER:HB3	1.92	0.50
1:B:96:ASP:OD1	1:B:97:THR:N	2.35	0.50
1:A:266:VAL:O	1:A:267:GLU:HG2	2.10	0.50
1:A:198:PRO:CG	1:A:230:LEU:HD11	2.42	0.50
1:A:11:THR:HG22	1:A:40:HIS:HB2	1.94	0.50
1:A:143:LEU:HD23	1:A:161:VAL:HG22	1.93	0.49
1:A:149:SER:HB3	1:A:290:ASN:HD21	1.78	0.49
1:B:9:ILE:O	1:B:38:LYS:HA	2.13	0.49
1:B:327:ARG:O	1:B:331:VAL:HG23	2.13	0.49
3:B:402:A2G:C7	3:B:403:A2G:H6	2.43	0.48
1:A:217:LYS:NZ	1:A:217:LYS:HB3	2.28	0.48
1:A:182:LYS:NZ	1:A:279:PHE:O	2.34	0.48
1:A:35:SER:HA	1:A:53:LYS:O	2.13	0.48
1:B:305:VAL:HG23	1:B:306:GLY:O	2.14	0.48
1:B:134:ARG:HD2	1:B:157:PHE:CD2	2.48	0.48
1:B:182:LYS:NZ	1:B:255:GLU:O	2.30	0.48
1:A:200:MSE:HE1	1:A:305:VAL:HG21	1.94	0.48
1:A:342:GLU:CG	1:A:344:SER:OG	2.60	0.48
1:A:92:ILE:HG23	1:A:114:ILE:HB	1.96	0.48
1:B:165:LEU:HD12	1:B:340:ASP:O	2.13	0.48
1:A:222:GLY:O	1:A:245:GLY:HA2	2.14	0.48
1:A:41:THR:HG21	1:A:59:GLN:HE21	1.79	0.48
1:B:133:ARG:HG3	1:B:137:TYR:CE1	2.47	0.48
1:B:324:GLU:CD	1:B:327:ARG:NH1	2.39	0.48
1:B:289:TYR:CE2	1:B:290:ASN:HB2	2.48	0.47
1:B:312:ALA:O	1:B:316:LYS:HG2	2.13	0.47
1:A:188:PHE:CD2	1:A:220:ILE:HG23	2.45	0.47
1:A:297:LYS:HB3	1:A:300:HIS:HB3	1.97	0.47
1:A:269:LEU:HG	1:A:274:ILE:HD11	1.96	0.47
1:B:172:ASP:OD2	1:B:343:ILE:HD12	2.14	0.47
1:B:254:TYR:HE1	1:B:260:LEU:HD13	1.80	0.47
1:A:289:TYR:CD2	1:A:290:ASN:HB2	2.50	0.47
1:A:118:HIS:HA	1:A:146:LEU:HD12	1.97	0.47
1:A:18:GLU:O	1:A:22:VAL:HG23	2.15	0.47
1:A:7:PHE:HB2	1:A:36:ILE:HG12	1.95	0.47
1:B:64:THR:HG22	1:B:66:TYR:H	1.80	0.47
1:A:298:ASP:HB2	1:A:304:LEU:HD12	1.96	0.46
1:A:202:LEU:HD13	1:A:234:VAL:HG23	1.98	0.46
1:A:320:VAL:HG12	1:A:321:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:TYR:CD2	1:B:290:ASN:HB2	2.51	0.46
1:A:114:ILE:O	1:A:115:ILE:CG1	2.63	0.46
1:A:29:CYS:SG	1:A:51:GLU:HB2	2.56	0.46
1:A:121:GLU:O	1:A:130:ARG:NH1	2.46	0.46
1:A:27:ALA:HB1	1:A:347:LYS:HE2	1.98	0.46
1:A:174:ILE:HD11	1:A:251:LYS:HE2	1.97	0.45
1:B:103:ILE:O	1:B:107:ILE:HG13	2.17	0.45
1:B:5:ILE:HD12	1:B:354:ILE:HD13	1.98	0.45
1:A:149:SER:O	1:A:152:VAL:HG22	2.17	0.45
1:B:343:ILE:HG13	1:B:343:ILE:H	1.54	0.45
1:A:94:PHE:O	1:A:95:LEU:HB2	2.17	0.45
1:B:14:SER:OG	1:B:14:SER:O	2.25	0.45
1:B:7:PHE:HB3	1:B:21:LEU:HD11	1.99	0.45
1:B:76:PHE:CZ	1:B:105:ALA:HA	2.51	0.45
1:B:188:PHE:HD1	1:B:220:ILE:HG23	1.82	0.45
1:A:63:ASP:O	1:A:67:HIS:HB2	2.17	0.44
1:A:327:ARG:O	1:A:331:VAL:HG23	2.17	0.44
1:B:90:VAL:HG23	1:B:112:PRO:HB2	1.98	0.44
1:B:174:ILE:HD11	1:B:251:LYS:HE2	2.00	0.44
1:A:112:PRO:HB3	1:A:357:VAL:HG12	2.00	0.44
1:B:212:LEU:HD11	1:B:318:GLU:HG3	2.00	0.44
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.70	0.44
1:A:12:LEU:HA	1:A:18:GLU:HG2	1.99	0.44
1:A:184:ASN:HB3	1:A:216:TYR:CG	2.53	0.44
1:A:200:MSE:HE2	1:A:313:LEU:HB2	1.99	0.43
1:B:219:VAL:HG22	1:B:242:ASP:HB2	2.00	0.43
3:B:403:A2G:N2	4:B:404:NDG:H4	2.33	0.43
1:B:262:LEU:HD22	1:B:273:LEU:HG	2.01	0.43
1:B:25:ALA:O	1:B:29:CYS:HB2	2.19	0.43
1:A:148:SER:O	1:A:152:VAL:HG13	2.19	0.43
1:A:289:TYR:CE2	1:A:290:ASN:HB2	2.54	0.42
1:B:132:LEU:HA	1:B:132:LEU:HD23	1.79	0.42
1:A:292:ALA:HB3	1:A:293:LYS:HZ2	1.82	0.42
1:A:26:ASN:OD1	1:A:49:GLU:HB2	2.20	0.42
1:A:85:GLU:CG	1:A:85:GLU:O	2.62	0.42
1:B:198:PRO:CG	1:B:230:LEU:HD11	2.49	0.42
2:A:401:UDN:C1'	3:A:402:A2G:O4	2.68	0.42
1:B:95:LEU:HD21	1:B:118:HIS:HB2	2.02	0.42
1:A:213:GLN:OE1	1:A:239:ILE:HG22	2.20	0.42
1:A:298:ASP:OD1	1:A:303:LEU:HA	2.20	0.42
1:A:80:ARG:HG3	1:A:105:ALA:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASN:HD22	1:B:122:ALA:HB3	1.85	0.42
1:B:13:ASN:O	1:B:15:GLY:N	2.53	0.42
1:B:27:ALA:HB1	1:B:347:LYS:HE2	2.01	0.42
1:B:72:ARG:HA	1:B:72:ARG:HD2	1.77	0.42
1:B:262:LEU:HA	1:B:262:LEU:HD12	1.77	0.41
1:A:192:LEU:HD13	1:A:230:LEU:HD12	2.01	0.41
1:B:185:LEU:HD12	1:B:217:LYS:O	2.20	0.41
1:A:114:ILE:O	1:A:115:ILE:HG12	2.20	0.41
1:A:36:ILE:HD12	1:A:52:VAL:HG11	2.02	0.41
1:A:261:CYS:HA	1:A:284:ILE:O	2.20	0.41
1:B:164:LEU:HD13	1:B:350:TRP:CE2	2.55	0.41
1:B:73:PHE:N	1:B:73:PHE:CD1	2.88	0.41
1:B:269:LEU:HA	1:B:269:LEU:HD12	1.81	0.41
1:A:120:ASN:ND2	1:A:122:ALA:H	2.19	0.41
1:A:213:GLN:HB2	1:A:213:GLN:HE21	1.61	0.41
1:A:45:PHE:CZ	1:A:248:GLU:HG2	2.56	0.41
1:B:217:LYS:HZ3	1:B:217:LYS:HB3	1.85	0.41
1:B:21:LEU:HD12	1:B:94:PHE:CD1	2.56	0.41
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.78	0.41
1:B:192:LEU:HD12	1:B:227:ARG:HB2	2.03	0.41
1:A:172:ASP:OD2	1:A:343:ILE:HD12	2.21	0.40
1:A:61:ARG:HD3	1:B:45:PHE:CD1	2.56	0.40
1:B:187:LEU:HA	1:B:187:LEU:HD23	1.68	0.40
1:A:317:LEU:HA	1:A:317:LEU:HD12	1.85	0.40
1:A:329:GLU:O	1:A:330:LEU:C	2.60	0.40
1:A:48:LEU:HD12	1:A:49:GLU:H	1.86	0.40
1:B:12:LEU:HD23	1:B:12:LEU:HA	1.91	0.40
1:B:169:HIS:HA	1:B:343:ILE:HD11	2.03	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	358/373 (96%)	316 (88%)	35 (10%)	7 (2%)	9	39
1	B	358/373 (96%)	310 (87%)	41 (12%)	7 (2%)	9	39
All	All	716/746 (96%)	626 (87%)	76 (11%)	14 (2%)	9	39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	115	ILE
1	B	115	ILE
1	A	340	ASP
1	B	14	SER
1	B	96	ASP
1	A	124	LEU
1	A	245	GLY
1	A	290	ASN
1	B	245	GLY
1	B	246	ARG
1	B	290	ASN
1	B	107	ILE
1	A	107	ILE

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	324/332 (98%)	318 (98%)	6 (2%)	62	81
1	B	324/332 (98%)	309 (95%)	15 (5%)	31	67
All	All	648/664 (98%)	627 (97%)	21 (3%)	44	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	96	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	TYR
1	A	152	VAL
1	A	227	ARG
1	A	320	VAL
1	B	20	VAL
1	B	38	LYS
1	B	89	ASP
1	B	115	ILE
1	B	123	TYR
1	B	128	THR
1	B	145	VAL
1	B	152	VAL
1	B	177	ASP
1	B	227	ARG
1	B	234	VAL
1	B	254	TYR
1	B	270	PRO
1	B	317	LEU
1	B	344	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	120	ASN
1	A	213	GLN
1	A	290	ASN
1	A	332	ASN
1	A	345	ASN
1	B	120	ASN
1	B	213	GLN
1	B	332	ASN

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 ⓘ

10 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	UDN	A	401	-	35,41,41	3.43	14 (40%)	40,62,62	2.71	13 (32%)
3	A2G	A	402	3	14,14,15	2.69	7 (50%)	15,19,21	2.09	8 (53%)
3	A2G	A	403	3,4	14,14,15	2.59	5 (35%)	15,19,21	1.61	4 (26%)
4	NDG	A	404	3,5	14,14,15	2.65	8 (57%)	15,19,21	2.04	5 (33%)
5	BUE	A	405	4	9,10,28	2.65	2 (22%)	9,15,37	1.57	2 (22%)
2	UDN	B	401	-	35,41,41	3.27	12 (34%)	40,62,62	2.85	15 (37%)
3	A2G	B	402	3	14,14,15	2.68	7 (50%)	15,19,21	1.59	4 (26%)
3	A2G	B	403	3,4	14,14,15	2.33	6 (42%)	15,19,21	2.44	6 (40%)
4	NDG	B	404	3,5	14,14,15	2.73	7 (50%)	15,19,21	3.10	9 (60%)
5	BUE	B	405	4	9,10,28	2.44	2 (22%)	9,15,37	1.28	2 (22%)

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	UDN	A	401	-	-	0/20/63/63	0/3/3/3
3	A2G	A	402	3	-	0/6/23/26	0/1/1/1
3	A2G	A	403	3,4	-	0/6/23/26	0/1/1/1
4	NDG	A	404	3,5	-	0/6/23/26	0/1/1/1
5	BUE	A	405	4	-	0/10/10/31	0/0/0/0
2	UDN	B	401	-	-	0/20/63/63	0/3/3/3
3	A2G	B	402	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2G	B	403	3,4	-	0/6/23/26	0/1/1/1
4	NDG	B	404	3,5	-	0/6/23/26	0/1/1/1
5	BUE	B	405	4	-	0/10/10/31	0/0/0/0

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	UDN	O4D-C1D	-8.77	1.29	1.41
2	A	401	UDN	O4D-C1D	-8.20	1.29	1.41
2	A	401	UDN	C5D-C4D	-7.88	1.26	1.51
2	A	401	UDN	PB-CB	-7.81	1.68	1.80
2	B	401	UDN	PB-CB	-7.80	1.68	1.80
2	B	401	UDN	C2D-C1D	-7.18	1.42	1.53
2	A	401	UDN	C2D-C1D	-6.51	1.43	1.53
2	A	401	UDN	C3D-C2D	-5.52	1.38	1.53
2	B	401	UDN	O3D-C3D	-5.39	1.30	1.43
2	B	401	UDN	PB-O2B	-4.33	1.45	1.56
2	A	401	UDN	O5D-C5D	-4.25	1.27	1.44
2	A	401	UDN	PB-O2B	-4.22	1.46	1.56
3	B	402	A2G	C6-C5	-3.15	1.41	1.51
3	A	402	A2G	C6-C5	-3.12	1.41	1.51
4	B	404	NDG	C6-C5	-3.04	1.41	1.51
4	A	404	NDG	C6-C5	-2.94	1.41	1.51
4	B	404	NDG	C1-C2	-2.93	1.48	1.52
2	A	401	UDN	PB-O1B	-2.68	1.44	1.51
2	B	401	UDN	O2'-C2D	-2.39	1.37	1.43
3	A	402	A2G	C3-C2	-2.32	1.47	1.52
2	B	401	UDN	C5D-C4D	-2.32	1.44	1.51
2	A	401	UDN	O2'-C2D	-2.29	1.37	1.43
4	B	404	NDG	C3-C2	-2.19	1.47	1.52
2	B	401	UDN	PB-O1B	-2.18	1.46	1.51
3	B	403	A2G	C3-C2	-2.16	1.47	1.52
3	B	402	A2G	C3-C2	-2.11	1.47	1.52
4	A	404	NDG	C1-C2	-2.09	1.49	1.52
4	A	404	NDG	C3-C2	-2.08	1.47	1.52
2	B	401	UDN	C2'-N2'	2.05	1.49	1.45
3	B	403	A2G	O-C5	2.07	1.47	1.43
3	A	402	A2G	O3-C3	2.16	1.47	1.43
3	B	403	A2G	C2-N2	2.16	1.50	1.46
3	A	403	A2G	O-C5	2.25	1.48	1.43
4	A	404	NDG	O-C1	2.26	1.47	1.43
2	A	401	UDN	O4D-C4D	2.47	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A2G	O3-C3	2.54	1.48	1.43
2	B	401	UDN	C7'-N2'	2.55	1.43	1.34
2	B	401	UDN	O5'-C5'	2.71	1.50	1.44
4	B	404	NDG	O3-C3	2.78	1.49	1.43
3	A	403	A2G	C2-N2	2.87	1.51	1.46
3	A	402	A2G	O-C1	2.94	1.48	1.43
3	B	402	A2G	O-C1	2.95	1.48	1.43
2	A	401	UDN	O5'-C5'	2.95	1.51	1.44
2	A	401	UDN	C7'-N2'	3.02	1.45	1.34
4	A	404	NDG	O3-C3	3.06	1.50	1.43
2	A	401	UDN	C2'-N2'	3.08	1.50	1.45
3	B	403	A2G	O-C1	3.19	1.48	1.43
5	A	405	BUE	P35-O36	3.28	1.68	1.54
5	B	405	BUE	P35-O36	3.33	1.68	1.54
4	A	404	NDG	C7-N2	3.37	1.46	1.34
3	B	403	A2G	C7-N2	3.42	1.46	1.34
4	B	404	NDG	C7-N2	3.44	1.47	1.34
3	A	403	A2G	O-C1	3.64	1.49	1.43
3	B	402	A2G	C7-N2	3.73	1.48	1.34
3	A	402	A2G	C7-N2	3.79	1.48	1.34
3	A	403	A2G	C7-N2	3.86	1.48	1.34
4	A	404	NDG	C2-N2	3.91	1.53	1.46
4	B	404	NDG	C2-N2	4.02	1.53	1.46
3	B	402	A2G	C2-N2	4.65	1.54	1.46
3	A	402	A2G	C2-N2	4.82	1.54	1.46
3	B	402	A2G	O-C5	5.05	1.54	1.43
3	A	402	A2G	O-C5	5.05	1.54	1.43
3	B	403	A2G	O6-C6	5.22	1.64	1.42
4	A	404	NDG	O-C5	5.43	1.54	1.43
5	B	405	BUE	P35-O38	5.57	1.69	1.60
4	B	404	NDG	O-C5	5.59	1.55	1.43
3	A	403	A2G	O6-C6	6.18	1.68	1.42
5	A	405	BUE	P35-O38	6.34	1.70	1.60
2	A	401	UDN	PB-O3A	6.72	1.66	1.58
2	B	401	UDN	PB-O3A	8.62	1.68	1.58

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	UDN	O4D-C4D-C3D	-5.84	93.55	105.17
3	B	403	A2G	C1-O-C5	-5.36	104.78	112.17
4	B	404	NDG	O-C1-C2	-4.78	104.82	111.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	A2G	O6-C6-C5	-4.50	96.19	111.34
4	B	404	NDG	O3-C3-C2	-4.47	99.81	109.39
4	B	404	NDG	O3-C3-C4	-4.39	100.80	110.36
4	B	404	NDG	C6-C5-C4	-4.03	103.58	113.00
2	B	401	UDN	C2D-C3D-C4D	-3.86	95.10	102.62
5	A	405	BUE	O37-P35-O34	-3.43	97.09	110.50
3	A	403	A2G	O6-C6-C5	-3.43	99.81	111.34
3	B	403	A2G	O-C1-C2	-3.31	106.87	111.47
4	A	404	NDG	O3-C3-C2	-3.08	102.78	109.39
2	B	401	UDN	O2B-PB-O1B	-2.98	100.13	110.09
4	A	404	NDG	O3-C3-C4	-2.97	103.90	110.36
5	A	405	BUE	O40-P39-O41	-2.83	97.62	112.28
3	A	402	A2G	C6-C5-C4	-2.80	106.44	113.00
3	B	403	A2G	C4-C3-C2	-2.78	106.94	111.02
2	B	401	UDN	C1'-C2'-N2'	-2.74	104.46	110.62
3	A	403	A2G	O-C1-C2	-2.68	107.74	111.47
2	B	401	UDN	C6'-C5'-C4'	-2.66	106.78	113.00
3	A	402	A2G	O4-C4-C5	-2.65	102.61	109.28
2	A	401	UDN	O2B-PB-O1B	-2.58	101.46	110.09
2	B	401	UDN	PA-O3A-PB	-2.55	124.17	132.39
5	B	405	BUE	O40-P39-O41	-2.53	99.18	112.28
2	B	401	UDN	C4D-O4D-C1D	-2.51	107.09	109.77
5	B	405	BUE	O37-P35-O34	-2.51	100.69	110.50
2	A	401	UDN	PA-O3A-PB	-2.46	124.46	132.39
3	B	403	A2G	C3-C4-C5	-2.36	106.05	110.22
3	A	402	A2G	O3-C3-C4	-2.22	105.53	110.36
2	B	401	UDN	O1A-PA-O2A	-2.17	101.05	112.28
2	B	401	UDN	O6'-C6'-C5'	-2.10	104.29	111.34
3	A	403	A2G	C3-C4-C5	-2.09	106.53	110.22
3	B	402	A2G	C1-C2-N2	-2.08	106.93	110.49
4	B	404	NDG	O4-C4-C5	-2.08	104.03	109.28
4	B	404	NDG	C2-N2-C7	-2.05	119.95	122.94
2	A	401	UDN	O2'-C2D-C3D	2.02	118.30	111.83
3	A	402	A2G	C4-C3-C2	2.04	114.00	111.02
2	A	401	UDN	O3D-C3D-C2D	2.12	118.63	111.83
3	B	402	A2G	C8-C7-N2	2.19	120.07	116.11
3	A	402	A2G	C8-C7-N2	2.24	120.16	116.11
4	A	404	NDG	C4-C3-C2	2.30	114.40	111.02
2	A	401	UDN	O1B-PB-CB	2.31	114.94	108.75
3	B	402	A2G	C1-O-C5	2.33	115.38	112.17
4	A	404	NDG	C8-C7-N2	2.48	120.58	116.11
2	B	401	UDN	O2'-C2D-C1D	2.52	119.50	111.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A2G	O-C1-C2	2.60	115.09	111.47
2	B	401	UDN	O2B-PB-CB	2.67	111.81	105.62
4	B	404	NDG	C8-C7-N2	2.78	121.12	116.11
3	A	403	A2G	C1-C2-N2	2.87	115.40	110.49
2	A	401	UDN	C4'-C3'-C2'	2.90	114.63	110.33
4	B	404	NDG	C4-C3-C2	2.92	115.30	111.02
3	B	403	A2G	C1-C2-N2	3.00	115.62	110.49
3	A	402	A2G	C1-O-C5	3.15	116.51	112.17
3	A	402	A2G	C3-C4-C5	3.32	116.06	110.22
2	B	401	UDN	O4D-C4D-C5D	3.32	120.61	109.40
2	A	401	UDN	O2B-PB-CB	3.34	113.36	105.62
2	B	401	UDN	O2'-C2D-C3D	3.42	122.78	111.83
3	B	402	A2G	O-C1-C2	3.78	116.73	111.47
4	A	404	NDG	C3-C4-C5	4.18	117.59	110.22
2	A	401	UDN	O2'-C2D-C1D	4.49	125.65	111.61
2	A	401	UDN	O4D-C4D-C5D	4.56	124.81	109.40
4	B	404	NDG	C3-C4-C5	5.52	119.95	110.22
2	A	401	UDN	O4D-C1D-N1	5.80	119.70	108.08
2	A	401	UDN	O3D-C3D-C4D	6.67	130.56	111.09
2	B	401	UDN	O3D-C3D-C4D	7.22	132.18	111.09
2	B	401	UDN	C4-N3-C2	8.32	121.27	114.13
2	A	401	UDN	C4-N3-C2	8.34	121.30	114.13
2	B	401	UDN	O4D-C1D-N1	8.76	125.63	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UDN	3	0
3	A	402	A2G	1	0
3	A	403	A2G	5	0
4	A	404	NDG	1	0
2	B	401	UDN	2	0
3	B	402	A2G	3	0
3	B	403	A2G	6	0
4	B	404	NDG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	356/373 (95%)	-0.45	0 100 100	48, 64, 88, 106	0
1	B	356/373 (95%)	-0.41	0 100 100	48, 69, 89, 107	0
All	All	712/746 (95%)	-0.43	0 100 100	48, 67, 89, 107	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	A2G	A	403	14/15	0.90	0.28	1.16	122,124,127,128	0
3	A2G	B	403	14/15	0.89	0.23	0.76	126,128,130,130	0
2	UDN	A	401	39/39	0.94	0.20	0.30	80,87,94,96	0
2	UDN	B	401	39/39	0.92	0.20	0.28	94,96,99,99	0
3	A2G	A	402	14/15	0.90	0.21	0.13	124,126,128,129	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	A2G	B	402	14/15	0.89	0.16	-0.45	126,129,132,132	0
5	BUE	A	405	11/29	0.90	0.14	-1.57	128,131,132,133	0
5	BUE	B	405	11/29	0.88	0.11	-3.76	134,139,145,146	0
4	NDG	B	404	14/15	0.82	0.15	-	129,131,132,132	0
4	NDG	A	404	14/15	0.85	0.18	-	124,127,129,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.