



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID : 3QKW
Title : Structure of Streptococcus parasanguini Gtf3 glycosyltransferase
Authors : Zhu, F.; Erlandsen, H.; Huang, Y.; Ding, L.; Zhou, M.; Liang, X.; Ma, J.-B.;
Wu, H.
Deposited on : 2011-02-01
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

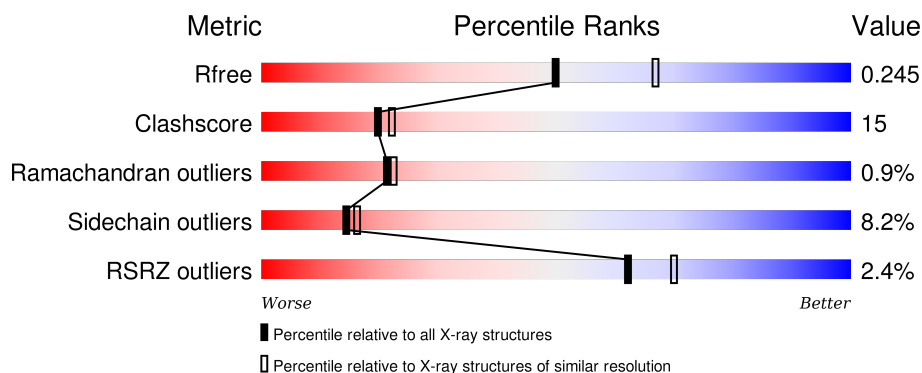
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	332	<div> <div>2%</div> <div>69% 25% 5%</div> </div>
1	B	332	<div> <div>2%</div> <div>75% 20%</div> </div>
1	C	332	<div> <div>2%</div> <div>70% 23% 5%</div> </div>
1	D	332	<div> <div>4%</div> <div>68% 27%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10871 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.

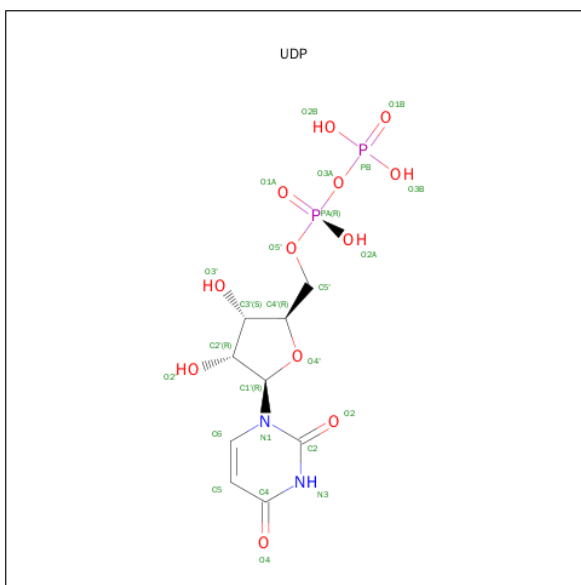
- Molecule 1 is a protein called Nucleotide sugar synthetase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2657	1708	443	490	16			
1	B	324	Total	C	N	O	S	0	0	0
			2618	1687	437	477	17			
1	C	329	Total	C	N	O	S	0	0	0
			2669	1717	443	492	17			
1	D	326	Total	C	N	O	S	0	0	0
			2639	1697	441	485	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	EXPRESSION TAG	UNP B5A7L9
A	0	CYS	-	EXPRESSION TAG	UNP B5A7L9
B	-1	ALA	-	EXPRESSION TAG	UNP B5A7L9
B	0	CYS	-	EXPRESSION TAG	UNP B5A7L9
C	-1	ALA	-	EXPRESSION TAG	UNP B5A7L9
C	0	CYS	-	EXPRESSION TAG	UNP B5A7L9
D	-1	ALA	-	EXPRESSION TAG	UNP B5A7L9
D	0	CYS	-	EXPRESSION TAG	UNP B5A7L9

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



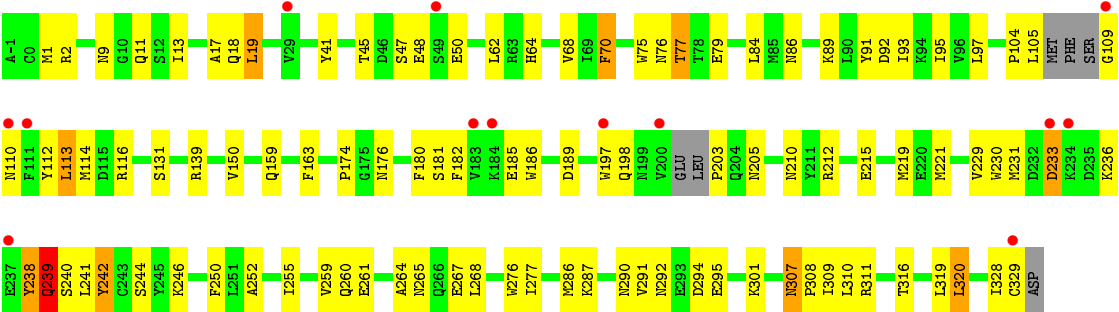
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	B	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	C	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	D	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	52	Total O 52 52	0	0
3	B	57	Total O 57 57	0	0
3	C	47	Total O 47 47	0	0
3	D	32	Total O 32 32	0	0



● Molecule 1: Nucleotide sugar synthetase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.22Å 99.24Å 188.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.51 – 2.29 42.51 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.7 (42.51-2.29) 95.7 (42.51-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_351)	Depositor
R, R_{free}	0.187 , 0.250 0.186 , 0.245	Depositor DCC
R_{free} test set	3218 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 63257 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10871	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/2716	0.59	2/3677 (0.1%)
1	B	0.49	0/2677	0.58	0/3625
1	C	0.40	0/2729	0.55	0/3693
1	D	0.38	0/2697	0.58	1/3649 (0.0%)
All	All	0.42	0/10819	0.58	3/14644 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ASP	N-CA-C	5.68	126.34	111.00
1	A	311	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	152	GLY	N-CA-C	5.23	126.18	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2657	0	2647	93	0
1	B	2618	0	2617	75	0
1	C	2669	0	2654	76	0
1	D	2639	0	2630	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	11	0	0
2	B	25	0	11	0	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
3	A	52	0	0	3	0
3	B	57	0	0	1	0
3	C	47	0	0	0	0
3	D	32	0	0	2	0
All	All	10871	0	10592	317	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 (317) 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:292:ASN:OD1	1:A:295:GLU:HG3	1.24	1.27
1:B:263:ILE:O	1:B:263:ILE:HD13	1.40	1.19
1:C:212:ARG:HB2	1:C:212:ARG:HH11	1.05	1.15
1:A:292:ASN:CG	1:A:295:GLU:HG3	1.75	1.06
1:D:64:HIS:HD2	1:D:92:ASP:H	1.10	0.99
1:D:231:MET:HG3	1:D:239:GLN:HB3	1.47	0.97
1:D:77:THR:HG22	1:D:79:GLU:H	1.26	0.97
1:C:64:HIS:HD2	1:C:92:ASP:H	1.13	0.96
1:C:212:ARG:HB2	1:C:212:ARG:NH1	1.81	0.93
1:B:263:ILE:C	1:B:263:ILE:HD13	1.83	0.91
1:B:11:GLN:H	1:B:18:GLN:HE22	1.16	0.90
1:A:240:SER:O	1:A:264:ALA:HB2	1.73	0.89
1:A:292:ASN:OD1	1:A:295:GLU:CG	2.17	0.87
1:A:317:ARG:HD2	3:A:371:HOH:O	1.75	0.87
1:C:77:THR:HG22	1:C:79:GLU:H	1.40	0.86
1:D:105:LEU:HB3	1:D:238:TYR:HE1	1.41	0.85
1:A:152:GLY:O	1:A:153:MET:HB2	1.79	0.82
1:D:291:VAL:HG23	1:D:295:GLU:HG3	1.61	0.81
1:A:11:GLN:H	1:A:18:GLN:HE22	1.26	0.80
1:B:251:LEU:O	1:B:307:ASN:ND2	2.13	0.79
1:B:297:ILE:O	1:B:301:LYS:HG2	1.83	0.79
1:D:64:HIS:CD2	1:D:92:ASP:H	1.98	0.78
1:D:316:THR:HG22	1:D:320:LEU:HD22	1.65	0.77
1:D:113:LEU:HD12	3:D:356:HOH:O	1.83	0.77
1:D:11:GLN:H	1:D:18:GLN:HE22	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLN:H	1:C:18:GLN:HE22	1.32	0.76
1:A:234:LYS:HB3	1:A:234:LYS:HZ2	1.49	0.75
1:B:262:GLY:H	1:B:266:GLN:HE22	1.32	0.75
1:B:263:ILE:O	1:B:263:ILE:CD1	2.30	0.74
1:B:179:ARG:HH21	1:B:231:MET:HE1	1.53	0.74
1:B:316:THR:HG22	1:B:320:LEU:HD22	1.69	0.74
1:A:234:LYS:H	1:A:234:LYS:HD2	1.51	0.74
1:C:202:LEU:HB2	1:C:203:PRO:HD2	1.70	0.74
1:B:263:ILE:HD11	1:B:266:GLN:HB3	1.69	0.73
1:C:75:TRP:HH2	1:C:106:MET:HE3	1.52	0.72
1:A:155:ASP:HB3	1:A:157:PRO:HD3	1.69	0.72
1:B:263:ILE:CD1	1:B:263:ILE:C	2.54	0.71
1:A:316:THR:HG22	1:A:320:LEU:HD22	1.72	0.71
1:A:56:ASP:OD1	1:A:87:LYS:HE3	1.89	0.71
1:D:105:LEU:HB3	1:D:238:TYR:CE1	2.25	0.71
1:A:230:TRP:CZ3	1:A:260:GLN:HG2	2.25	0.71
1:C:212:ARG:CB	1:C:212:ARG:HH11	1.95	0.71
1:B:202:LEU:HD12	1:B:208:LYS:HB2	1.73	0.70
1:A:156:HIS:HE1	1:A:214:ASP:OD2	1.74	0.70
1:A:216:GLN:O	1:A:220:GLU:HG3	1.91	0.70
1:C:103:VAL:HG23	1:C:106:MET:HE2	1.75	0.69
1:C:103:VAL:HG12	1:C:104:PRO:HD3	1.75	0.68
1:B:179:ARG:NH2	1:B:231:MET:CE	2.56	0.68
1:B:315:PHE:O	3:B:336:HOH:O	2.11	0.68
1:A:231:MET:HG2	1:A:239:GLN:HB2	1.77	0.67
1:C:13:ILE:HD12	1:C:13:ILE:H	1.60	0.67
1:B:76:ASN:O	1:B:77:THR:HB	1.95	0.67
1:C:202:LEU:CB	1:C:203:PRO:HD2	2.26	0.66
1:A:158:THR:HG21	1:A:218:LEU:HD23	1.77	0.66
1:A:236:LYS:O	1:A:239:GLN:HB3	1.96	0.66
1:D:238:TYR:O	1:D:241:LEU:N	2.24	0.66
1:A:238:TYR:HD2	1:A:238:TYR:O	1.78	0.66
1:A:152:GLY:O	1:A:268:LEU:CD1	2.44	0.66
1:A:172:HIS:HD2	1:A:195:TYR:OH	1.77	0.66
1:B:240:SER:CB	1:B:263:ILE:HA	2.26	0.66
1:B:179:ARG:NH2	1:B:231:MET:HE1	2.10	0.66
1:C:307:ASN:C	1:C:307:ASN:HD22	1.99	0.66
1:C:106:MET:HB3	1:C:238:TYR:CE1	2.31	0.65
1:B:240:SER:HB3	1:B:263:ILE:HA	1.79	0.65
1:C:307:ASN:HD22	1:C:308:PRO:HD3	1.61	0.65
1:C:316:THR:HG22	1:C:320:LEU:HD22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ILE:CD1	1:B:266:GLN:HB3	2.27	0.64
1:D:307:ASN:HD22	1:D:308:PRO:HD3	1.62	0.64
1:D:70:PHE:CZ	1:D:84:LEU:HD23	2.33	0.64
1:D:76:ASN:O	1:D:77:THR:HB	1.96	0.64
1:D:17:ALA:HB1	1:D:75:TRP:CZ3	2.32	0.64
1:A:230:TRP:CH2	1:A:260:GLN:HG2	2.32	0.64
1:A:11:GLN:HB2	1:A:18:GLN:NE2	2.13	0.64
1:A:290:ASN:O	1:A:291:VAL:C	2.37	0.63
1:B:172:HIS:HD2	1:B:195:TYR:OH	1.80	0.63
1:C:212:ARG:HG2	1:C:216:GLN:CD	2.19	0.63
1:C:210:ASN:O	1:C:212:ARG:HD3	1.98	0.63
1:B:263:ILE:HD12	1:B:263:ILE:N	2.14	0.62
1:B:239:GLN:O	1:B:241:LEU:N	2.28	0.62
1:C:156:HIS:HE1	1:C:214:ASP:OD2	1.81	0.62
1:A:199:ASN:H	1:A:199:ASN:HD22	1.48	0.62
1:A:158:THR:HG21	1:A:218:LEU:CD2	2.30	0.62
1:C:76:ASN:O	1:C:77:THR:HB	2.00	0.61
1:B:137:LYS:HB2	1:B:137:LYS:NZ	2.15	0.61
1:B:307:ASN:CB	1:B:308:PRO:HD3	2.30	0.61
1:C:102:VAL:HG11	1:C:105:LEU:HD12	1.81	0.61
1:A:292:ASN:ND2	1:A:295:GLU:HG3	2.15	0.61
1:C:64:HIS:CD2	1:C:92:ASP:H	2.05	0.61
1:B:76:ASN:O	1:B:77:THR:CB	2.48	0.61
1:C:135:ILE:O	1:C:139:ARG:HG2	2.00	0.61
1:A:156:HIS:N	1:A:157:PRO:HD3	2.16	0.61
1:C:179:ARG:HH21	1:C:231:MET:CE	2.14	0.60
1:C:307:ASN:HD22	1:C:308:PRO:CD	2.14	0.60
1:B:239:GLN:OE1	1:B:239:GLN:HA	2.01	0.60
1:A:70:PHE:CZ	1:A:84:LEU:HD23	2.37	0.60
1:A:307:ASN:HD22	1:A:307:ASN:C	2.04	0.60
1:D:104:PRO:O	1:D:105:LEU:HG	2.01	0.60
1:D:11:GLN:HB2	1:D:18:GLN:NE2	2.16	0.60
1:D:11:GLN:HB2	1:D:18:GLN:HE21	1.66	0.60
1:D:233:ASP:HA	1:D:236:LYS:HG3	1.83	0.59
1:A:307:ASN:HD22	1:A:308:PRO:HD3	1.68	0.59
1:D:197:TRP:CD1	1:D:198:GLN:HG3	2.37	0.59
1:D:292:ASN:OD1	1:D:295:GLU:HG2	2.03	0.58
1:D:186:TRP:HB3	1:D:203:PRO:HG3	1.84	0.58
1:D:221:MET:HE1	1:D:255:ILE:HD11	1.85	0.58
1:A:159:GLN:HB2	3:A:358:HOH:O	2.03	0.58
1:D:221:MET:CE	1:D:255:ILE:HD11	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LYS:HA	1:D:239:GLN:HG2	1.85	0.57
1:D:64:HIS:HD2	1:D:92:ASP:N	1.91	0.57
1:D:104:PRO:HG3	1:D:114:MET:HA	1.87	0.57
1:D:105:LEU:CB	1:D:238:TYR:HE1	2.15	0.57
1:D:131:SER:HA	1:D:150:VAL:HG13	1.86	0.57
1:A:133:LYS:HG2	1:A:241:LEU:HD12	1.86	0.57
1:A:262:GLY:H	1:A:266:GLN:HE22	1.53	0.57
1:B:11:GLN:HB2	1:B:18:GLN:HE21	1.69	0.56
1:C:179:ARG:HH21	1:C:231:MET:HE1	1.71	0.56
1:B:11:GLN:HB2	1:B:18:GLN:NE2	2.21	0.56
1:A:157:PRO:HA	1:A:311:ARG:O	2.05	0.56
1:C:76:ASN:O	1:C:77:THR:CB	2.54	0.56
1:D:89:LYS:HD3	1:D:95:ILE:HD12	1.88	0.56
1:C:176:ASN:HB3	1:C:198:GLN:HE21	1.71	0.56
1:D:229:VAL:HB	1:D:259:VAL:HG12	1.87	0.56
1:D:186:TRP:HB3	1:D:203:PRO:CG	2.36	0.55
1:C:143:MET:HE3	1:C:145:VAL:H	1.71	0.55
1:D:238:TYR:O	1:D:240:SER:N	2.39	0.55
1:A:307:ASN:HD22	1:A:308:PRO:CD	2.20	0.55
1:D:316:THR:O	1:D:320:LEU:HB2	2.07	0.55
1:B:179:ARG:NH2	1:B:231:MET:HE2	2.22	0.55
1:D:197:TRP:NE1	1:D:198:GLN:HG3	2.22	0.55
1:A:265:ASN:ND2	3:A:352:HOH:O	2.39	0.55
1:D:11:GLN:H	1:D:18:GLN:NE2	2.04	0.54
1:D:307:ASN:HD22	1:D:308:PRO:CD	2.21	0.54
1:D:261:GLU:HA	1:D:277:ILE:CG2	2.37	0.54
1:D:231:MET:CG	1:D:239:GLN:HB3	2.31	0.54
1:C:307:ASN:HD22	1:C:308:PRO:N	2.06	0.54
1:B:11:GLN:H	1:B:18:GLN:NE2	1.97	0.54
1:A:11:GLN:H	1:A:18:GLN:NE2	2.00	0.54
1:D:112:TYR:N	3:D:356:HOH:O	2.41	0.54
1:A:172:HIS:HE1	1:A:224:GLY:O	1.91	0.54
1:D:286:MET:HG2	1:D:290:ASN:HD21	1.73	0.54
1:D:77:THR:HG22	1:D:79:GLU:N	2.09	0.53
1:B:294:ASP:HA	1:B:297:ILE:HD12	1.90	0.53
1:B:11:GLN:N	1:B:18:GLN:HE22	1.95	0.53
1:A:156:HIS:N	1:A:157:PRO:CD	2.69	0.53
1:B:200:VAL:HG12	1:B:201:GLU:O	2.08	0.53
1:C:176:ASN:HB3	1:C:198:GLN:NE2	2.24	0.53
1:B:103:VAL:O	1:B:106:MET:HG3	2.08	0.53
1:A:127:VAL:HG23	1:A:145:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:NZ	1:A:234:LYS:HB3	2.22	0.52
1:B:9:ASN:ND2	1:B:10:GLY:H	2.06	0.52
1:D:238:TYR:O	1:D:239:GLN:C	2.48	0.52
1:A:139:ARG:HG3	1:A:139:ARG:HH11	1.74	0.52
1:D:91:TYR:HB3	1:D:93:ILE:HG23	1.90	0.52
1:A:234:LYS:H	1:A:234:LYS:CD	2.20	0.52
1:B:263:ILE:CD1	1:B:263:ILE:N	2.70	0.52
1:A:137:LYS:HG3	1:A:141:PHE:HE2	1.75	0.52
1:B:293:GLU:O	1:B:297:ILE:HD12	2.09	0.52
1:A:9:ASN:ND2	1:B:63:ARG:HE	2.08	0.51
1:B:284:ALA:O	1:B:288:VAL:HG23	2.11	0.51
1:D:221:MET:HE3	1:D:250:PHE:CE1	2.46	0.51
1:C:107:PHE:HB3	1:C:110:ASN:HD22	1.76	0.51
1:A:137:LYS:HE2	1:A:141:PHE:CZ	2.46	0.51
1:D:76:ASN:O	1:D:77:THR:CB	2.58	0.50
1:A:172:HIS:HB3	1:A:221:MET:HE1	1.93	0.50
1:C:307:ASN:ND2	1:C:308:PRO:HD3	2.25	0.50
1:A:133:LYS:HG2	1:A:241:LEU:CD1	2.41	0.50
1:D:181:SER:O	1:D:185:GLU:HG2	2.11	0.50
1:B:213:PRO:HD2	1:B:216:GLN:HE21	1.75	0.50
1:B:70:PHE:CD1	1:B:70:PHE:C	2.85	0.50
1:C:307:ASN:ND2	1:C:307:ASN:C	2.63	0.50
1:A:217:LEU:HD11	1:A:221:MET:CE	2.42	0.50
1:A:290:ASN:O	1:A:291:VAL:O	2.30	0.50
1:A:293:GLU:O	1:A:297:ILE:HG12	2.12	0.50
1:C:89:LYS:HD3	1:C:95:ILE:HD12	1.94	0.50
1:A:13:ILE:O	1:A:13:ILE:HD13	2.11	0.50
1:A:156:HIS:O	1:A:157:PRO:C	2.51	0.49
1:A:291:VAL:O	1:A:291:VAL:HG13	2.12	0.49
1:A:11:GLN:HB2	1:A:18:GLN:HE21	1.77	0.49
1:C:107:PHE:HB3	1:C:110:ASN:ND2	2.28	0.49
1:A:53:LYS:HE3	1:B:54:ARG:NH2	2.27	0.49
1:B:217:LEU:O	1:B:221:MET:HG3	2.12	0.49
1:A:233:ASP:O	1:A:236:LYS:HB2	2.12	0.49
1:A:238:TYR:O	1:A:238:TYR:CD2	2.62	0.49
1:C:75:TRP:CH2	1:C:106:MET:HE3	2.40	0.49
1:A:307:ASN:ND2	1:A:307:ASN:C	2.66	0.49
1:B:9:ASN:ND2	1:B:10:GLY:N	2.61	0.49
1:C:204:GLN:HG3	1:C:205:ASN:N	2.28	0.49
1:C:53:LYS:HD2	1:D:50:GLU:HB3	1.95	0.49
1:A:53:LYS:HE3	1:B:54:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HD3	1:A:143:MET:O	2.12	0.48
1:D:180:PHE:HB3	1:D:182:PHE:CE1	2.48	0.48
1:D:252:ALA:O	1:D:311:ARG:NH1	2.41	0.48
1:A:82:GLU:OE2	1:A:116:ARG:HB3	2.13	0.48
1:C:240:SER:OG	1:C:241:LEU:HD13	2.14	0.48
1:D:319:LEU:C	1:D:319:LEU:HD12	2.33	0.48
1:A:292:ASN:CG	1:A:295:GLU:CG	2.66	0.48
1:B:213:PRO:HD2	1:B:216:GLN:NE2	2.28	0.48
1:B:186:TRP:CE3	1:B:192:LEU:HD22	2.49	0.48
1:D:264:ALA:O	1:D:265:ASN:HB2	2.13	0.48
1:C:212:ARG:NH2	1:C:220:GLU:OE1	2.47	0.48
1:A:152:GLY:O	1:A:268:LEU:HD11	2.14	0.47
1:C:214:ASP:OD2	1:C:218:LEU:HD22	2.15	0.47
1:A:202:LEU:HB3	1:A:203:PRO:HD2	1.96	0.47
1:C:70:PHE:C	1:C:70:PHE:CD1	2.87	0.47
1:D:176:ASN:HB3	1:D:198:GLN:OE1	2.15	0.47
1:C:9:ASN:ND2	1:C:10:GLY:H	2.12	0.47
1:B:246:LYS:HG2	1:B:250:PHE:CE2	2.50	0.47
1:C:133:LYS:HD3	1:C:133:LYS:N	2.28	0.47
1:D:47:SER:OG	1:D:50:GLU:HG3	2.15	0.47
1:D:242:TYR:CD2	1:D:242:TYR:C	2.87	0.47
1:D:1:MET:SD	1:D:328:ILE:HD11	2.55	0.46
1:A:72:THR:OG1	1:A:73:PRO:HA	2.15	0.46
1:A:307:ASN:HD22	1:A:308:PRO:N	2.13	0.46
1:A:307:ASN:N	1:A:308:PRO:CD	2.77	0.46
1:C:4:TYR:HB2	1:C:68:VAL:HG22	1.96	0.46
1:B:179:ARG:HH21	1:B:231:MET:CE	2.21	0.46
1:C:216:GLN:O	1:C:220:GLU:HG3	2.15	0.46
1:D:109:GLY:HA2	1:D:110:ASN:HA	1.78	0.46
1:B:212:ARG:HB2	1:B:216:GLN:NE2	2.31	0.46
1:B:262:GLY:O	1:B:263:ILE:O	2.34	0.46
1:A:156:HIS:CD2	1:A:249:SER:OG	2.69	0.46
1:C:242:TYR:CD1	1:C:242:TYR:C	2.89	0.46
1:C:207:HIS:N	1:C:207:HIS:CD2	2.83	0.46
1:C:283:GLU:O	1:C:287:LYS:HG3	2.16	0.46
1:C:232:ASP:N	1:C:232:ASP:OD1	2.46	0.45
1:B:307:ASN:CB	1:B:308:PRO:CD	2.94	0.45
1:C:212:ARG:HG2	1:C:216:GLN:NE2	2.32	0.45
1:D:113:LEU:HD23	1:D:116:ARG:HH11	1.81	0.45
1:B:13:ILE:N	1:B:13:ILE:HD13	2.31	0.45
1:C:56:ASP:OD1	1:C:87:LYS:NZ	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLU:OE1	1:C:237:GLU:HA	2.16	0.45
1:D:189:ASP:HA	1:D:205:ASN:ND2	2.32	0.45
1:A:130:PRO:HA	1:A:151:GLN:HE21	1.82	0.45
1:A:328:ILE:HG21	1:D:309:ILE:HG13	1.98	0.45
1:C:70:PHE:C	1:C:70:PHE:HD1	2.20	0.45
1:A:11:GLN:N	1:A:18:GLN:HE22	2.04	0.45
1:D:89:LYS:HA	1:D:89:LYS:HD2	1.76	0.45
1:D:112:TYR:CD2	1:D:113:LEU:HG	2.52	0.45
1:B:139:ARG:HG3	1:B:139:ARG:HH11	1.81	0.45
1:A:234:LYS:N	1:A:234:LYS:HZ3	2.13	0.45
1:A:242:TYR:C	1:A:242:TYR:CD1	2.88	0.45
1:B:262:GLY:H	1:B:266:GLN:NE2	2.06	0.44
1:A:195:TYR:HA	1:A:209:ILE:O	2.17	0.44
1:A:217:LEU:HD11	1:A:221:MET:HE3	1.99	0.44
1:C:307:ASN:N	1:C:308:PRO:CD	2.80	0.44
1:B:82:GLU:OE2	1:B:116:ARG:HB3	2.16	0.44
1:D:319:LEU:HD12	1:D:320:LEU:N	2.32	0.44
1:D:307:ASN:C	1:D:307:ASN:HD22	2.19	0.44
1:A:292:ASN:ND2	1:A:295:GLU:CG	2.80	0.44
1:B:307:ASN:HB2	1:B:308:PRO:HD3	1.99	0.44
1:C:103:VAL:CG1	1:C:104:PRO:HD3	2.45	0.44
1:A:236:LYS:NZ	1:A:260:GLN:HE22	2.16	0.44
1:B:139:ARG:HD3	1:B:143:MET:O	2.17	0.44
1:A:12:SER:C	1:A:14:GLN:H	2.21	0.44
1:B:216:GLN:HG3	1:D:219:MET:HE1	1.99	0.44
1:D:45:THR:O	1:D:45:THR:HG22	2.16	0.44
1:D:19:LEU:HD22	1:D:19:LEU:HA	1.65	0.44
1:C:161:PRO:HD2	1:C:219:MET:SD	2.58	0.44
1:D:113:LEU:HD23	1:D:116:ARG:NH1	2.33	0.44
1:C:143:MET:HE3	1:C:145:VAL:N	2.32	0.44
1:A:63:ARG:HE	1:B:9:ASN:ND2	2.16	0.44
1:C:202:LEU:CB	1:C:203:PRO:CD	2.95	0.44
1:D:174:PRO:HD2	1:D:246:LYS:HD3	2.00	0.44
1:A:299:LEU:O	1:A:303:VAL:HG23	2.18	0.43
1:A:9:ASN:HD21	1:B:63:ARG:HE	1.66	0.43
1:C:62:LEU:HD23	1:C:62:LEU:HA	1.88	0.43
1:A:256:PRO:HB3	1:A:299:LEU:HB3	2.00	0.43
1:C:294:ASP:O	1:C:297:ILE:HB	2.19	0.43
1:C:89:LYS:HA	1:C:89:LYS:HD2	1.85	0.43
1:C:153:MET:CE	1:C:268:LEU:HD23	2.49	0.43
1:C:55:LEU:O	1:C:59:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD12	1:C:253:ALA:HB2	2.00	0.43
1:D:13:ILE:H	1:D:13:ILE:HG13	1.50	0.43
1:B:262:GLY:O	1:B:263:ILE:C	2.57	0.43
1:A:287:LYS:HE3	1:A:287:LYS:HB3	1.86	0.43
1:A:199:ASN:HD22	1:A:199:ASN:N	2.15	0.43
1:C:300:VAL:O	1:C:304:ARG:HG3	2.19	0.42
1:C:77:THR:HG22	1:C:79:GLU:N	2.20	0.42
1:B:172:HIS:CD2	1:B:195:TYR:OH	2.67	0.42
1:B:264:ALA:O	1:B:265:ASN:HB2	2.18	0.42
1:B:137:LYS:HZ3	1:B:137:LYS:HB2	1.84	0.42
1:B:215:GLU:OE1	1:D:215:GLU:OE1	2.37	0.42
1:D:139:ARG:HH11	1:D:139:ARG:HG2	1.84	0.42
1:C:262:GLY:H	1:C:266:GLN:HE22	1.66	0.42
1:A:319:LEU:C	1:A:319:LEU:HD12	2.39	0.42
1:A:156:HIS:CE1	1:A:214:ASP:OD2	2.63	0.42
1:D:230:TRP:CH2	1:D:260:GLN:HG3	2.55	0.41
1:B:70:PHE:HD1	1:B:70:PHE:C	2.22	0.41
1:A:128:VAL:HG22	1:A:149:VAL:HB	2.02	0.41
1:A:309:ILE:HG22	1:A:310:LEU:N	2.35	0.41
1:D:104:PRO:O	1:D:105:LEU:CG	2.68	0.41
1:A:12:SER:C	1:A:14:GLN:N	2.74	0.41
1:C:11:GLN:H	1:C:18:GLN:NE2	2.09	0.41
1:B:172:HIS:HE1	1:B:224:GLY:O	2.03	0.41
1:B:309:ILE:HD11	1:C:329:CYS:HB2	2.03	0.41
1:D:104:PRO:HA	1:D:110:ASN:O	2.21	0.41
1:B:277:ILE:HD12	1:B:277:ILE:N	2.35	0.41
1:B:128:VAL:HG22	1:B:149:VAL:HB	2.02	0.41
1:D:62:LEU:HD21	1:D:68:VAL:HG21	2.01	0.41
1:C:63:ARG:HE	1:D:9:ASN:ND2	2.18	0.41
1:A:230:TRP:CE3	1:A:260:GLN:HG2	2.55	0.41
1:D:197:TRP:CD1	1:D:198:GLN:N	2.89	0.41
1:D:221:MET:HE1	1:D:250:PHE:HD1	1.85	0.41
1:D:215:GLU:O	1:D:219:MET:HG3	2.21	0.41
1:A:14:GLN:HG2	1:A:197:TRP:CZ3	2.56	0.41
1:D:291:VAL:CG2	1:D:295:GLU:HG3	2.43	0.41
1:B:176:ASN:HA	1:B:177:PRO:HD3	1.77	0.41
1:C:180:PHE:HB3	1:C:182:PHE:CE1	2.56	0.41
1:D:276:TRP:CD2	1:D:287:LYS:HD3	2.56	0.41
1:C:190:ILE:HA	1:C:191:PRO:HD3	1.90	0.40
1:D:221:MET:CE	1:D:250:PHE:CD1	3.04	0.40
1:D:238:TYR:C	1:D:240:SER:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASN:HD22	1:B:10:GLY:H	1.69	0.40
1:C:206:VAL:C	1:C:207:HIS:HD2	2.24	0.40
1:C:86:ASN:HA	1:C:86:ASN:HD22	1.64	0.40
1:B:216:GLN:NE2	1:D:163:PHE:HZ	2.20	0.40
1:B:252:ALA:O	1:B:311:ARG:NH1	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	324/332 (98%)	308 (95%)	12 (4%)	4 (1%)	16	15
1	B	320/332 (96%)	308 (96%)	8 (2%)	4 (1%)	15	14
1	C	325/332 (98%)	316 (97%)	7 (2%)	2 (1%)	30	34
1	D	320/332 (96%)	304 (95%)	14 (4%)	2 (1%)	30	34
All	All	1289/1328 (97%)	1236 (96%)	41 (3%)	12 (1%)	21	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	VAL
1	B	77	THR
1	A	232	ASP
1	B	240	SER
1	B	263	ILE
1	C	77	THR
1	D	77	THR
1	A	157	PRO
1	D	239	GLN
1	C	307	ASN

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Mol	Chain	Res	Type
1	B	203	PRO
1	A	307	ASN

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	295/298 (99%)	270 (92%)	25 (8%)	13	15
1	B	290/298 (97%)	274 (94%)	16 (6%)	27	34
1	C	296/298 (99%)	264 (89%)	32 (11%)	8	8
1	D	292/298 (98%)	269 (92%)	23 (8%)	15	17
All	All	1173/1192 (98%)	1077 (92%)	96 (8%)	14	16

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	13	ILE
1	A	14	GLN
1	A	70	PHE
1	A	97	LEU
1	A	98	PHE
1	A	120	TYR
1	A	134	MET
1	A	138	LEU
1	A	178	GLU
1	A	199	ASN
1	A	208	LYS
1	A	210	ASN
1	A	212	ARG
1	A	233	ASP
1	A	234	LYS
1	A	235	ASP
1	A	238	TYR
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	242	TYR
1	A	305	SER
1	A	307	ASN
1	A	310	LEU
1	A	320	LEU
1	A	329	CYS
1	B	2	ARG
1	B	12	SER
1	B	70	PHE
1	B	97	LEU
1	B	98	PHE
1	B	120	TYR
1	B	137	LYS
1	B	241	LEU
1	B	244	SER
1	B	246	LYS
1	B	263	ILE
1	B	268	LEU
1	B	281	VAL
1	B	307	ASN
1	B	310	LEU
1	B	320	LEU
1	C	2	ARG
1	C	19	LEU
1	C	30	SER
1	C	70	PHE
1	C	97	LEU
1	C	105	LEU
1	C	107	PHE
1	C	120	TYR
1	C	133	LYS
1	C	138	LEU
1	C	143	MET
1	C	185	GLU
1	C	188	TYR
1	C	201	GLU
1	C	202	LEU
1	C	210	ASN
1	C	212	ARG
1	C	218	LEU
1	C	232	ASP
1	C	239	GLN

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Mol	Chain	Res	Type
1	C	241	LEU
1	C	242	TYR
1	C	244	SER
1	C	246	LYS
1	C	266	GLN
1	C	268	LEU
1	C	270	GLU
1	C	294	ASP
1	C	301	LYS
1	C	307	ASN
1	C	310	LEU
1	C	320	LEU
1	D	2	ARG
1	D	19	LEU
1	D	41	TYR
1	D	48	GLU
1	D	70	PHE
1	D	86	ASN
1	D	97	LEU
1	D	113	LEU
1	D	159	GLN
1	D	210	ASN
1	D	212	ARG
1	D	238	TYR
1	D	239	GLN
1	D	242	TYR
1	D	244	SER
1	D	267	GLU
1	D	268	LEU
1	D	294	ASP
1	D	301	LYS
1	D	307	ASN
1	D	310	LEU
1	D	320	LEU
1	D	329	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	18	GLN
1	A	22	ASN

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Mol	Chain	Res	Type
1	A	86	ASN
1	A	100	HIS
1	A	151	GLN
1	A	156	HIS
1	A	172	HIS
1	A	199	ASN
1	A	207	HIS
1	A	210	ASN
1	A	216	GLN
1	A	260	GLN
1	A	266	GLN
1	A	307	ASN
1	A	326	GLN
1	B	9	ASN
1	B	18	GLN
1	B	86	ASN
1	B	110	ASN
1	B	151	GLN
1	B	172	HIS
1	B	210	ASN
1	B	216	GLN
1	B	266	GLN
1	B	326	GLN
1	C	9	ASN
1	C	18	GLN
1	C	64	HIS
1	C	86	ASN
1	C	110	ASN
1	C	151	GLN
1	C	156	HIS
1	C	207	HIS
1	C	210	ASN
1	C	216	GLN
1	C	223	GLN
1	C	239	GLN
1	C	266	GLN
1	C	307	ASN
1	C	326	GLN
1	D	9	ASN
1	D	18	GLN
1	D	64	HIS
1	D	86	ASN

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Mol	Chain	Res	Type
1	D	151	GLN
1	D	239	GLN
1	D	266	GLN
1	D	290	ASN
1	D	307	ASN
1	D	326	GLN

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 ⓘ

4 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	UDP	A	400	-	18,26,26	1.19	1 (5%)	26,40,40	1.69	3 (11%)
2	UDP	B	400	-	18,26,26	1.26	1 (5%)	26,40,40	1.41	2 (7%)
2	UDP	C	400	-	18,26,26	1.19	1 (5%)	26,40,40	1.51	2 (7%)
2	UDP	D	400	-	18,26,26	1.17	1 (5%)	26,40,40	1.54	2 (7%)

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	UDP	A	400	-	-	0/12/32/32	0/2/2/2
2	UDP	B	400	-	-	0/12/32/32	0/2/2/2
2	UDP	C	400	-	-	0/12/32/32	0/2/2/2
2	UDP	D	400	-	-	0/12/32/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	UDP	C4-N3	2.51	1.37	1.33
2	C	400	UDP	C4-N3	2.93	1.38	1.33
2	D	400	UDP	C4-N3	3.01	1.38	1.33
2	B	400	UDP	C4-N3	3.14	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	UDP	PA-O3A-PB	-2.55	124.12	132.67
2	C	400	UDP	PA-O3A-PB	-2.50	124.29	132.67
2	A	400	UDP	PA-O3A-PB	-2.14	125.48	132.67
2	B	400	UDP	O4'-C1'-N1	2.36	113.06	108.08
2	A	400	UDP	O4'-C1'-N1	2.43	113.20	108.08
2	D	400	UDP	C4-N3-C2	5.60	119.69	114.14
2	B	400	UDP	C4-N3-C2	5.66	119.75	114.14
2	C	400	UDP	C4-N3-C2	5.90	119.99	114.14
2	A	400	UDP	C4-N3-C2	6.72	120.79	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	328/332 (98%)	-0.08	8 (2%) 62 70	27, 43, 82, 124	0
1	B	324/332 (97%)	-0.22	5 (1%) 76 81	20, 43, 73, 102	0
1	C	329/332 (99%)	-0.03	6 (1%) 71 77	28, 50, 91, 109	0
1	D	326/332 (98%)	0.11	13 (3%) 42 49	31, 53, 92, 122	0
All	All	1307/1328 (98%)	-0.06	32 (2%) 62 70	20, 47, 86, 124	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	200	VAL	6.2
1	A	239	GLN	4.4
1	C	197	TRP	3.5
1	D	183	VAL	3.4
1	A	262	GLY	3.3
1	D	329	CYS	3.3
1	A	234	LYS	3.1
1	C	202	LEU	3.0
1	D	234	LYS	2.9
1	A	152	GLY	2.8
1	B	231	MET	2.8
1	B	187	LYS	2.7
1	B	262	GLY	2.7
1	D	197	TRP	2.7
1	A	242	TYR	2.5
1	C	183	VAL	2.4
1	B	239	GLN	2.4
1	A	235	ASP	2.4
1	C	0	CYS	2.4
1	D	111	PHE	2.4
1	A	286	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	237	GLU	2.3
1	D	110	ASN	2.2
1	A	291	VAL	2.2
1	C	210	ASN	2.2
1	B	13	ILE	2.2
1	D	49	SER	2.2
1	D	109	GLY	2.1
1	D	184	LYS	2.1
1	C	211	TYR	2.1
1	D	233	ASP	2.1
1	D	29	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	UDP	D	400	25/25	0.98	0.11	-0.49	43,50,57,60	0
2	UDP	A	400	25/25	0.98	0.11	-0.51	29,38,51,56	0
2	UDP	B	400	25/25	0.98	0.10	-0.61	25,38,49,51	0
2	UDP	C	400	25/25	0.98	0.11	-0.66	39,51,63,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.