Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 11:52 AM EDT

PDB ID	:	5VIE
Title	:	Electrophilic probes for deciphering substrate recognition by O-GlcNAc transferase
Authors	:	Jiang, J.; Li, B.; Hu, C.-W.; Worth, M.; Fan, D.; Li, H.
Deposited on	:	2017-04-15
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

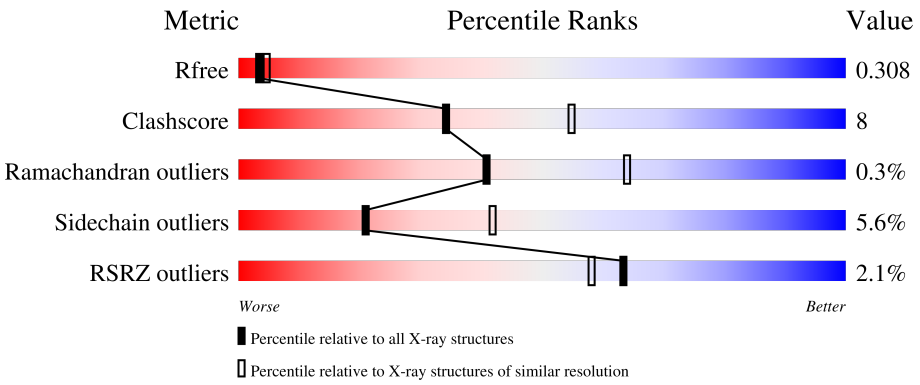
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	723	2%, 73%, 17%, •, 8%
1	C	723	2%, 73%, 17%, •, 8%
2	B	14	36%, 43%, 7%, 14%
2	D	14	57%, 29%, 14%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10972 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 UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5275	3356	915	967	37	0	3	0
1	C	667	5279	3358	914	971	36	0	2	0

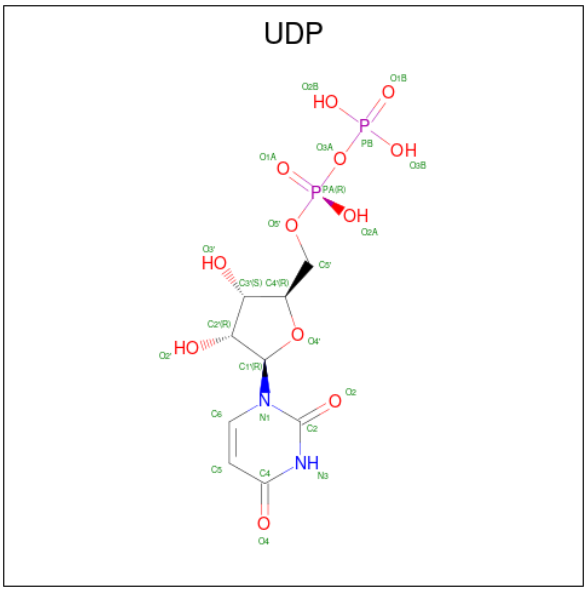
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLY	-	expression tag	UNP O15294
A	310	PRO	-	expression tag	UNP O15294
A	311	GLY	-	expression tag	UNP O15294
A	312	SER	-	expression tag	UNP O15294
C	309	GLY	-	expression tag	UNP O15294
C	310	PRO	-	expression tag	UNP O15294
C	311	GLY	-	expression tag	UNP O15294
C	312	SER	-	expression tag	UNP O15294

- Molecule 2 is a protein called CKII.

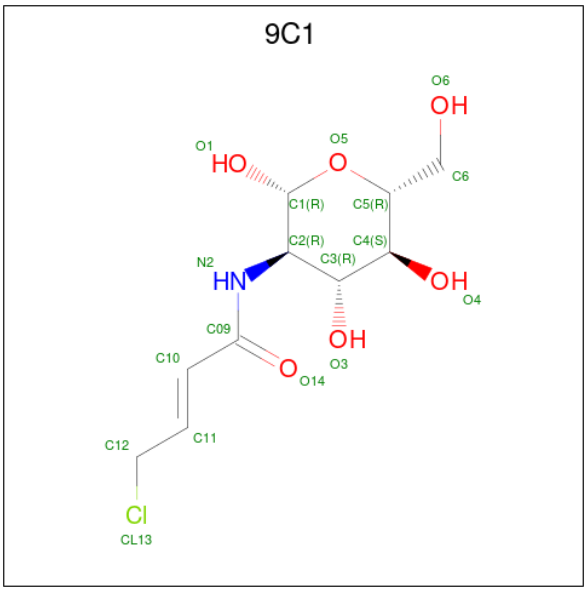
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	12	79	48	13	18	0	0	0
2	D	12	79	48	13	18	0	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



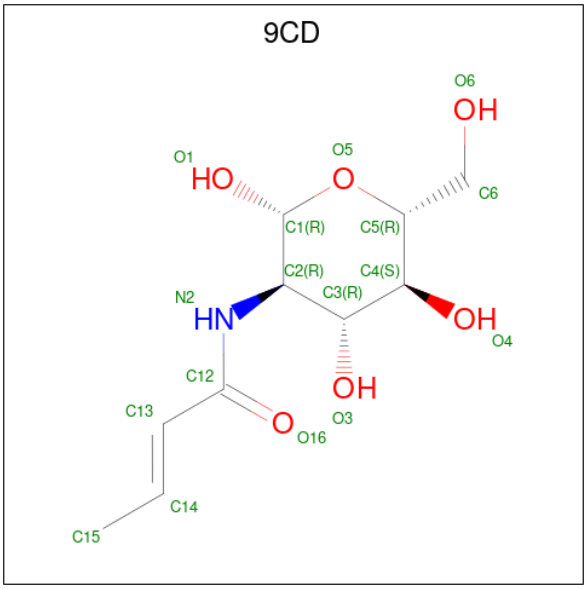
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	C	1	25	9	2	12	2	0	0

- Molecule 4 is 2-{[(2E)-4-chlorobut-2-enoyl]amino}-2-deoxy-beta-D-glucopyranose (three-letter code: 9C1) (formula: $C_{10}H_{16}ClNO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	B	1	17	10	1	1	5	0	0

- Molecule 5 is 2-{[(2E)-but-2-enoyl]amino}-2-deoxy-beta-D-glucopyranose (three-letter code: 9CD) (formula: $C_{10}H_{17}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	16	10	1	5	0	0

- Molecule 6 is water.

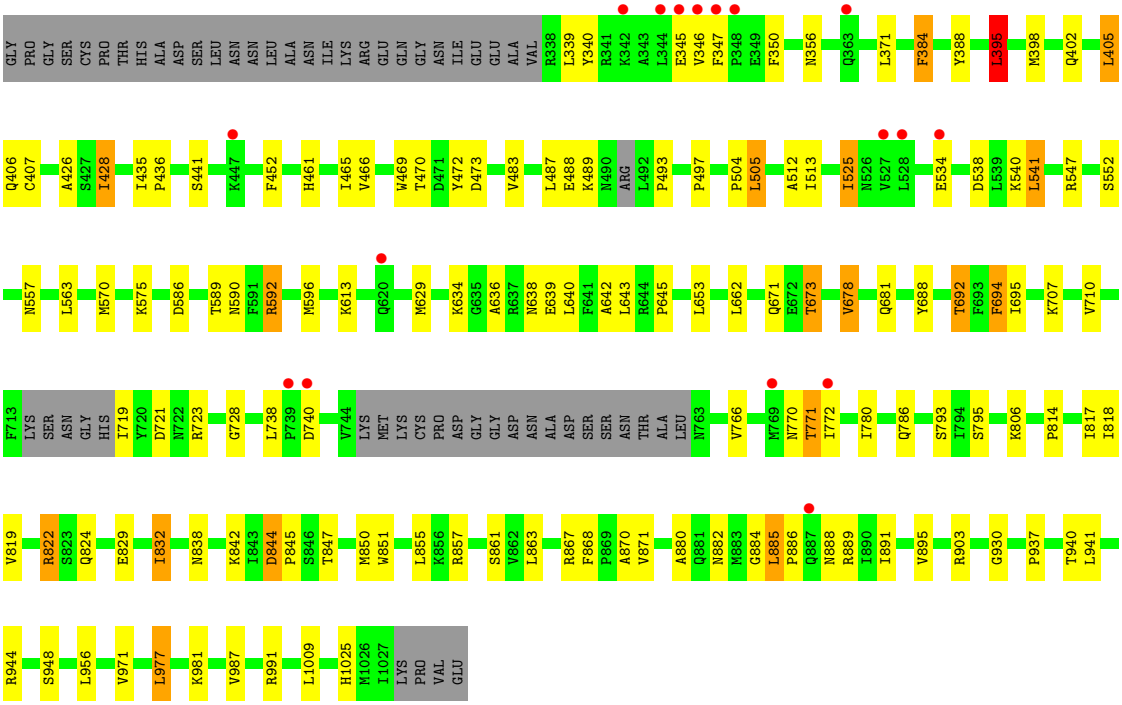
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	80	80	80	0	0
6	B	7	7	7	0	0
6	C	89	89	89	0	0
6	D	1	1	1	0	0

3 Residue-property plots (i)

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

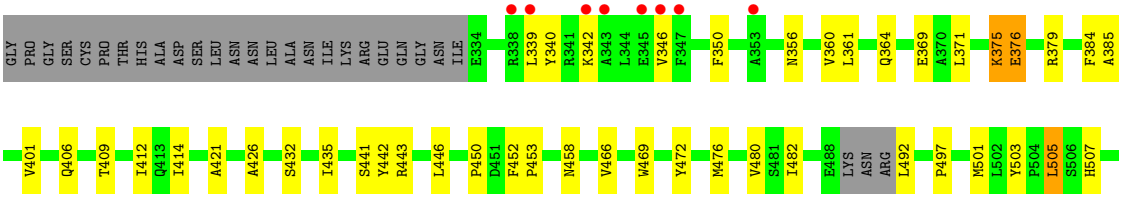
• Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

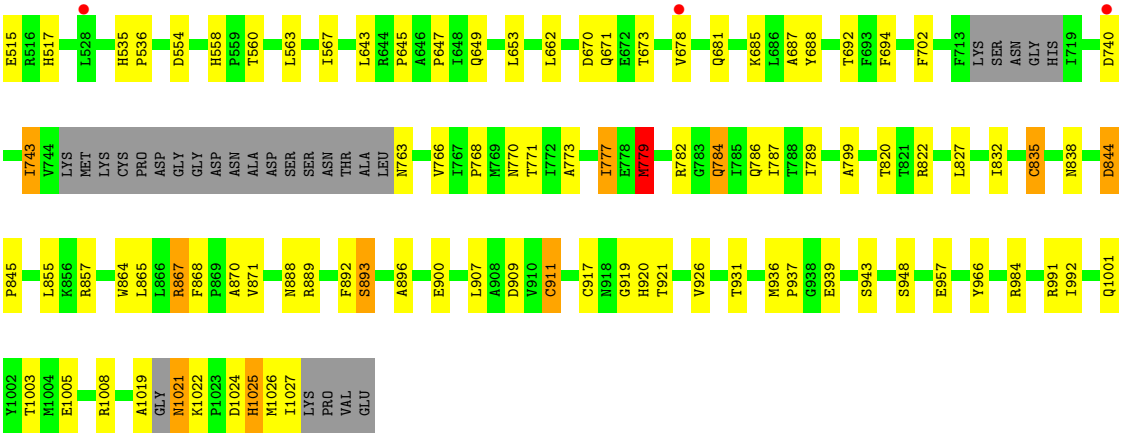
Chain A:



• Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

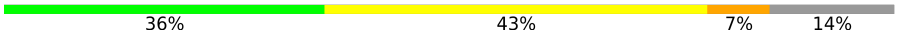
Chain C:

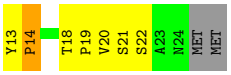




- Molecule 2: CKII

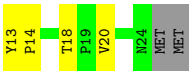
Chain B:





- Molecule 2: CKII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	138.73Å 200.03Å 152.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.60 47.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.01-2.60) 89.5 (47.26-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.248 , 0.308 0.248 , 0.308	Depositor DCC
R_{free} test set	2906 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5366e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 9C1, 9CD, 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	0.78	0/5408	0.94	8/7336 (0.1%)
1	C	0.79	0/5408	0.94	12/7338 (0.2%)
2	B	0.93	0/81	1.01	0/111
2	D	0.82	0/81	0.88	0/111
All	All	0.78	0/10978	0.94	20/14896 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	822	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	C	443	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	395	LEU	CB-CG-CD1	-7.25	98.68	111.00
1	C	857	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	991	ARG	CG-CD-NE	-6.71	97.71	111.80
1	C	339	LEU	CA-CB-CG	6.48	130.20	115.30
1	C	991	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	867	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	977	LEU	CA-CB-CG	6.25	129.67	115.30
1	C	991	ARG	NE-CZ-NH1	6.22	123.41	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	541	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	592	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	541	LEU	CB-CG-CD2	5.67	120.63	111.00
1	C	492	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	443	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	779	MET	CG-SD-CE	-5.36	91.62	100.20
1	C	702	PHE	C-N-CD	5.33	139.60	128.40
1	C	844	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	844	ASP	CB-CG-OD1	5.22	122.99	118.30
1	C	371	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	LEU	Peptide
1	C	835	CYS	Peptide

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	5275	0	5248	97	0
1	C	5279	0	5241	78	0
2	B	79	0	69	6	0
2	D	79	0	69	3	0
3	A	25	0	11	2	0
3	C	25	0	11	2	0
4	B	17	0	0	2	0
5	C	16	0	0	0	0
6	A	80	0	0	1	0
6	B	7	0	0	0	0
6	C	89	0	0	1	0
6	D	1	0	0	0	0
All	All	10972	0	10649	179	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 8.

All (179) 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)
4:B:101:9C1:C12	4:B:101:9C1:CL13	2.01	1.45
1:C:673:THR:HG22	1:C:948:SER:HB2	1.45	0.99
1:C:361:LEU:HD13	1:C:369:GLU:HG2	1.48	0.95
1:A:673:THR:HG22	1:A:941:LEU:HD12	1.53	0.90
1:A:861:SER:O	1:A:889:ARG:NH1	2.05	0.89
1:A:678:VAL:HG13	1:A:681:GLN:HE22	1.33	0.89
1:C:920:HIS:HB2	3:C:1101:UDP:O1B	1.73	0.87
1:A:673:THR:CG2	1:A:941:LEU:HD12	2.09	0.82
1:A:885:LEU:HD13	1:A:886:PRO:HD2	1.63	0.79
1:A:643:LEU:O	1:A:645:PRO:HD3	1.83	0.77
1:A:855:LEU:O	1:A:889:ARG:NH2	2.18	0.76
1:A:636:ALA:HB1	1:A:638:ASN:ND2	2.03	0.73
1:A:723:ARG:NH1	1:A:829:GLU:O	2.20	0.73
1:C:673:THR:CG2	1:C:948:SER:HB2	2.17	0.72
1:A:371:LEU:HD22	1:A:398:MET:HE1	1.73	0.71
1:A:525:ILE:HD13	1:A:643:LEU:HG	1.72	0.71
1:A:885:LEU:HB3	1:A:886:PRO:HD2	1.74	0.70
1:C:787:ILE:HD12	1:C:789:ILE:HD11	1.74	0.70
1:A:886:PRO:HG2	1:A:888:ASN:OD1	1.92	0.69
1:A:692:THR:HG23	1:A:948:SER:OG	1.94	0.68
1:A:525:ILE:HD12	1:A:642:ALA:HB3	1.76	0.67
1:C:779:MET:CE	1:C:787:ILE:HG23	2.24	0.67
2:B:13:TYR:N	2:B:18:THR:HG1	1.93	0.66
1:C:820:THR:HG22	1:C:907:LEU:HD21	1.78	0.66
1:A:940:THR:O	1:A:944:ARG:HG2	1.95	0.66
1:C:822:ARG:NH2	1:C:909:ASP:OD1	2.29	0.65
1:A:636:ALA:HB1	1:A:638:ASN:HD22	1.61	0.65
1:A:347:PHE:CD2	1:A:350:PHE:HB2	2.32	0.65
1:C:779:MET:HE1	1:C:787:ILE:HG23	1.78	0.65
1:A:525:ILE:HD11	1:A:639:GLU:O	1.96	0.64
2:D:13:TYR:N	2:D:18:THR:HG1	1.93	0.64
1:A:483:VAL:HG21	1:A:505:LEU:HD21	1.78	0.64
1:A:678:VAL:HG13	1:A:681:GLN:NE2	2.10	0.64
1:A:557:ASN:HB2	1:A:589:THR:HG21	1.81	0.63
1:A:885:LEU:CB	1:A:886:PRO:HD2	2.30	0.62
1:A:371:LEU:HD22	1:A:398:MET:CE	2.29	0.62
1:A:405:LEU:HG	1:A:428:ILE:HD11	1.82	0.62
1:C:844:ASP:HB2	1:C:845:PRO:HD2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASN:O	2:B:19:PRO:HG3	2.00	0.62
1:A:653:LEU:O	1:A:653:LEU:HG	1.98	0.61
1:A:586:ASP:OD1	1:A:592:ARG:HG2	2.02	0.60
1:A:592:ARG:O	1:A:596:MET:HG3	2.02	0.60
1:A:466:VAL:CG1	1:A:871:VAL:HG23	2.32	0.59
1:C:799:ALA:HA	6:C:1231:HOH:O	2.02	0.59
1:A:851:TRP:CE3	1:A:863:LEU:HD21	2.37	0.59
1:A:903:ARG:HG2	1:A:903:ARG:HH11	1.68	0.59
1:A:461:HIS:NE2	1:A:465:ILE:HD11	2.18	0.59
1:A:466:VAL:HG12	1:A:871:VAL:HG23	1.85	0.59
1:A:728:GLY:HA3	1:A:817:ILE:HG12	1.85	0.58
1:C:476:MET:O	1:C:480:VAL:HG23	2.03	0.58
1:A:483:VAL:HG21	1:A:505:LEU:CD2	2.35	0.57
1:C:507:HIS:HE1	1:C:939:GLU:HB3	1.69	0.56
1:C:779:MET:HA	1:C:784:GLN:HE21	1.69	0.56
1:A:723:ARG:HA	1:A:822:ARG:HG3	1.87	0.56
1:A:738:LEU:HD22	1:A:772:ILE:HG21	1.87	0.56
1:C:340:TYR:CZ	1:C:356:ASN:HB3	2.40	0.56
1:C:937:PRO:HA	1:C:943:SER:O	2.05	0.56
1:C:865:LEU:O	1:C:892:PHE:HA	2.05	0.56
1:C:1019:ALA:O	1:C:1021:ASN:N	2.39	0.56
1:C:469:TRP:O	1:C:472:TYR:HB2	2.05	0.56
1:A:681:GLN:OE1	1:A:681:GLN:N	2.35	0.56
1:C:687:ALA:HA	1:C:1026:MET:HB2	1.88	0.56
1:A:692:THR:HG22	1:A:694:PHE:H	1.71	0.55
1:C:835:CYS:SG	1:C:911:CYS:HB2	2.47	0.55
1:A:436:PRO:HG2	1:C:409:THR:HG21	1.87	0.55
1:C:412:ILE:HG13	1:C:421:ALA:HB1	1.89	0.54
1:C:685:LYS:HD3	1:C:1025:HIS:CE1	2.43	0.54
1:C:779:MET:HE1	1:C:786:GLN:C	2.28	0.53
1:C:673:THR:HG22	1:C:948:SER:CB	2.30	0.53
1:A:525:ILE:CD1	1:A:639:GLU:O	2.56	0.53
1:A:469:TRP:O	1:A:472:TYR:HB2	2.08	0.53
1:A:552:SER:HB2	1:A:629:MET:HB2	1.91	0.52
1:A:885:LEU:CD1	1:A:886:PRO:HD2	2.34	0.52
1:A:903:ARG:HG2	1:A:903:ARG:NH1	2.23	0.52
1:C:643:LEU:O	1:C:645:PRO:HD3	2.09	0.52
1:A:795:SER:O	1:A:819:VAL:HG12	2.09	0.52
1:C:453:PRO:HB3	1:C:482:ILE:HG23	1.92	0.52
1:A:855:LEU:HD22	1:A:889:ARG:NH1	2.25	0.52
3:C:1101:UDP:H5'1	2:D:20:VAL:HG12	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:TYR:O	1:A:1009:LEU:HD13	2.10	0.52
1:C:896:ALA:HB1	1:C:900:GLU:HB3	1.92	0.51
1:C:442:TYR:CZ	1:C:458:ASN:HB3	2.45	0.51
1:A:838:ASN:HB3	1:A:842:LYS:HD2	1.91	0.51
1:C:867:ARG:HB3	1:C:870:ALA:HB2	1.92	0.51
2:B:14:PRO:HG2	1:C:375:LYS:HZ2	1.76	0.51
1:C:678:VAL:HG12	1:C:681:GLN:HG3	1.94	0.50
1:C:507:HIS:N	1:C:507:HIS:CD2	2.79	0.50
1:A:371:LEU:HD21	2:D:14:PRO:O	2.12	0.49
1:C:926:VAL:HG22	1:C:931:THR:HB	1.94	0.49
1:A:426:ALA:HB2	1:A:441:SER:HB3	1.93	0.49
1:A:402:GLN:HG2	1:C:432:SER:O	2.12	0.49
1:C:554:ASP:HB2	1:C:560:THR:HB	1.95	0.49
1:C:838:ASN:HD21	1:C:919:GLY:HA2	1.78	0.48
1:A:388:TYR:O	1:A:407:CYS:HB3	2.13	0.48
1:C:446:LEU:O	1:C:450:PRO:HA	2.13	0.48
1:C:645:PRO:HD2	1:C:649:GLN:OE1	2.13	0.48
1:C:670:ASP:OD2	1:C:692:THR:HA	2.13	0.48
1:A:340:TYR:CZ	1:A:356:ASN:HB3	2.49	0.48
1:C:770:ASN:OD1	1:C:771:THR:N	2.35	0.48
1:C:501:MET:HE1	1:C:917:CYS:SG	2.54	0.47
1:C:466:VAL:HG12	1:C:871:VAL:HG23	1.96	0.47
1:A:832:ILE:O	1:A:861:SER:HA	2.15	0.47
1:C:673:THR:CG2	1:C:948:SER:CB	2.90	0.46
1:A:563:LEU:HD22	1:A:695:ILE:O	2.16	0.46
1:A:673:THR:HG21	1:A:941:LEU:HD12	1.95	0.46
1:A:895:VAL:HG13	3:A:1100:UDP:C4	2.51	0.46
1:C:501:MET:HE1	1:C:917:CYS:HB2	1.97	0.46
1:C:376:GLU:HG3	1:C:379:ARG:HH21	1.80	0.46
1:A:487:LEU:HD11	1:A:512:ALA:HB1	1.97	0.46
1:C:385:ALA:HB2	1:C:414:ILE:HG22	1.98	0.46
1:A:770:ASN:OD1	1:A:771:THR:N	2.38	0.46
1:C:855:LEU:O	1:C:889:ARG:NH2	2.49	0.45
1:C:936:MET:HB2	1:C:966:TYR:HD2	1.81	0.45
1:A:395:LEU:HA	1:A:398:MET:HE2	1.98	0.45
1:A:710:VAL:HG11	1:A:721:ASP:HA	1.98	0.45
1:A:487:LEU:HD21	1:A:512:ALA:CB	2.46	0.45
1:A:345:GLU:OE1	1:A:346:VAL:HG23	2.17	0.45
3:A:1100:UDP:H5'1	2:B:20:VAL:HG12	1.99	0.45
1:A:855:LEU:HD23	1:A:861:SER:OG	2.17	0.44
1:C:501:MET:HE3	1:C:501:MET:HB2	1.73	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:HIS:O	1:A:465:ILE:HG12	2.17	0.44
1:C:497:PRO:HD3	1:C:517:HIS:CE1	2.52	0.44
1:A:723:ARG:HD2	1:A:822:ARG:HD2	2.00	0.44
1:A:814:PRO:HD3	6:A:1246:HOH:O	2.17	0.44
1:A:671:GLN:HA	1:A:688:TYR:CZ	2.52	0.44
1:A:885:LEU:CB	1:A:886:PRO:CD	2.96	0.44
1:A:844:ASP:HB2	1:A:845:PRO:HD2	2.00	0.43
1:C:766:VAL:O	1:C:768:PRO:HD3	2.18	0.43
1:C:864:TRP:HE1	1:C:893:SER:HG	1.65	0.43
1:A:930:GLY:HA2	1:A:987:VAL:HG12	1.99	0.43
1:C:563:LEU:HD12	1:C:653:LEU:HD11	1.98	0.43
1:C:743:ILE:HD11	1:C:763:ASN:HB3	2.00	0.43
1:A:678:VAL:CG1	1:A:678:VAL:O	2.67	0.43
1:A:780:ILE:HD12	1:A:824:GLN:NE2	2.34	0.43
1:A:541:LEU:HD22	1:A:547:ARG:HH12	1.82	0.43
1:C:360:VAL:O	1:C:364:GLN:HG2	2.19	0.43
1:C:773:ALA:O	1:C:777:ILE:HG23	2.18	0.43
4:B:101:9C1:CL13	4:B:101:9C1:C11	2.97	0.43
1:A:487:LEU:HD21	1:A:512:ALA:HB3	2.00	0.42
1:A:738:LEU:CD2	1:A:772:ILE:HG21	2.48	0.42
1:C:688:TYR:HD2	1:C:1027:ILE:HG13	1.85	0.42
1:A:880:ALA:O	1:A:884:GLY:N	2.50	0.42
1:C:1001:GLN:O	1:C:1005:GLU:HG2	2.19	0.42
1:A:590:ASN:OD1	1:A:806:LYS:NZ	2.53	0.42
1:A:855:LEU:CD2	1:A:889:ARG:NH1	2.82	0.42
1:A:436:PRO:HG2	1:C:409:THR:CG2	2.50	0.42
1:A:538:ASP:OD2	1:A:540:LYS:HB2	2.20	0.42
1:A:634:LYS:N	2:B:22:SER:O	2.50	0.42
1:C:412:ILE:HG13	1:C:421:ALA:CB	2.49	0.42
1:A:493:PRO:HG2	1:A:513:ILE:HA	2.01	0.42
1:A:497:PRO:HG3	1:A:513:ILE:HG22	2.02	0.42
1:A:867:ARG:HB3	1:A:870:ALA:HA	2.02	0.42
1:C:426:ALA:HB2	1:C:441:SER:HB2	2.02	0.42
1:C:787:ILE:HD12	1:C:789:ILE:CD1	2.48	0.42
1:A:435:ILE:N	1:A:436:PRO:CD	2.83	0.42
1:A:340:TYR:CE1	1:A:356:ASN:HB3	2.55	0.41
1:C:535:HIS:HA	1:C:536:PRO:HD2	1.91	0.41
1:A:466:VAL:HG11	1:A:871:VAL:HG23	2.02	0.41
1:A:719:ILE:HD12	1:A:766:VAL:HG11	2.02	0.41
1:C:779:MET:HE3	1:C:787:ILE:HG23	1.99	0.41
1:A:857:ARG:HD3	1:A:971:VAL:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:LEU:HB3	1:A:886:PRO:CD	2.41	0.41
1:C:503:TYR:HB2	1:C:505:LEU:HD22	2.01	0.41
1:C:535:HIS:HB3	1:C:647:PRO:HD3	2.02	0.41
1:C:342:LYS:O	1:C:346:VAL:HG23	2.20	0.41
1:C:554:ASP:HB3	1:C:558:HIS:HB3	2.02	0.41
1:C:779:MET:HE1	1:C:787:ILE:N	2.35	0.41
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.84	0.41
1:A:723:ARG:HA	1:A:723:ARG:HD3	1.94	0.41
1:C:662:LEU:H	1:C:662:LEU:HD23	1.86	0.41
1:C:822:ARG:HB3	1:C:827:LEU:HB2	2.03	0.40
1:A:937:PRO:HB2	1:A:944:ARG:NH1	2.36	0.40
2:B:21:SER:O	2:B:22:SER:HB3	2.20	0.40
1:C:554:ASP:HB3	1:C:558:HIS:CG	2.56	0.40
1:C:563:LEU:HD21	1:C:921:THR:HG23	2.04	0.40
1:C:567:ILE:HG23	1:C:1003:THR:HG23	2.03	0.40
1:A:847:THR:HA	1:A:850[A]:MET:HE2	2.02	0.40
1:C:678:VAL:HG12	1:C:678:VAL:O	2.21	0.40
1:C:984:ARG:HG2	1:C:984:ARG:HH11	1.86	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	661/723 (91%)	622 (94%)	36 (5%)	3 (0%)	29 52
1	C	659/723 (91%)	623 (94%)	36 (6%)	0	100 100
2	B	10/14 (71%)	8 (80%)	1 (10%)	1 (10%)	0 0
2	D	10/14 (71%)	8 (80%)	2 (20%)	0	100 100
All	All	1340/1474 (91%)	1261 (94%)	75 (6%)	4 (0%)	41 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	PHE
1	A	882	ASN
1	A	504	PRO
2	B	14	PRO

5.3.2 Protein sidechains (i)

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	575/618 (93%)	540 (94%)	35 (6%)	18	38
1	C	575/618 (93%)	545 (95%)	30 (5%)	23	46
2	B	9/11 (82%)	9 (100%)	0	100	100
2	D	9/11 (82%)	9 (100%)	0	100	100
All	All	1168/1258 (93%)	1103 (94%)	65 (6%)	21	42

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	PHE
1	A	395	LEU
1	A	405	LEU
1	A	406	GLN
1	A	428	ILE
1	A	452	PHE
1	A	470	THR
1	A	473	ASP
1	A	488	GLU
1	A	489	LYS
1	A	505	LEU
1	A	525	ILE
1	A	534	GLU
1	A	570	MET
1	A	575	LYS
1	A	613	LYS
1	A	662	LEU
1	A	673	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	678	VAL
1	A	692	THR
1	A	694	PHE
1	A	707	LYS
1	A	740	ASP
1	A	771	THR
1	A	786	GLN
1	A	793	SER
1	A	818	ILE
1	A	832	ILE
1	A	868	PHE
1	A	885	LEU
1	A	891	ILE
1	A	956	LEU
1	A	977	LEU
1	A	981	LYS
1	A	1025	HIS
1	C	350	PHE
1	C	375	LYS
1	C	376	GLU
1	C	384	PHE
1	C	401	VAL
1	C	406	GLN
1	C	435	ILE
1	C	452	PHE
1	C	505	LEU
1	C	515	GLU
1	C	671	GLN
1	C	694	PHE
1	C	740	ASP
1	C	743	ILE
1	C	777	ILE
1	C	779	MET
1	C	782	ARG
1	C	784	GLN
1	C	832	ILE
1	C	868	PHE
1	C	888	ASN
1	C	893	SER
1	C	911	CYS
1	C	957	GLU
1	C	992	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1008	ARG
1	C	1021	ASN
1	C	1022	LYS
1	C	1024	ASP
1	C	1025	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	368	GLN
1	A	498	HIS
1	A	649	GLN
1	C	364	GLN
1	C	784	GLN
1	C	838	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	9C1	B	101	2	17,17,18	1.90	5 (29%)	18,22,24	2.55	10 (55%)
3	UDP	A	1100	-	24,26,26	1.03	1 (4%)	37,40,40	1.96	10 (27%)
5	9CD	C	1102	2,1	16,16,17	2.33	3 (18%)	18,21,23	1.55	3 (16%)
3	UDP	C	1101	-	24,26,26	1.82	3 (12%)	37,40,40	2.89	18 (48%)

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
4	9C1	B	101	2	-	1/9/27/30	0/1/1/1
3	UDP	A	1100	-	-	4/16/32/32	0/2/2/2
5	9CD	C	1102	2,1	-	4/9/26/29	0/1/1/1
3	UDP	C	1101	-	-	2/16/32/32	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1102	9CD	C1-C2	7.63	1.63	1.52
3	C	1101	UDP	C2-N1	5.87	1.47	1.38
4	B	101	9C1	C12-CL13	4.90	2.01	1.79
3	C	1101	UDP	C4-N3	-4.14	1.31	1.38
4	B	101	9C1	C10-C11	2.96	1.39	1.32
3	A	1100	UDP	C4-N3	-2.87	1.33	1.38
3	C	1101	UDP	O2-C2	2.77	1.28	1.23
5	C	1102	9CD	C3-C2	2.60	1.58	1.52
4	B	101	9C1	O5-C1	2.26	1.47	1.43
5	C	1102	9CD	O5-C1	2.25	1.47	1.43
4	B	101	9C1	C09-N2	2.11	1.39	1.34
4	B	101	9C1	C4-C5	2.00	1.57	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1101	UDP	C4-N3-C2	-8.07	115.94	126.58
3	C	1101	UDP	N3-C2-N1	5.77	122.55	114.89
3	C	1101	UDP	C5-C4-N3	5.38	122.89	114.84
4	B	101	9C1	C10-C09-N2	5.31	124.76	114.56
3	C	1101	UDP	O4-C4-N3	-5.13	111.77	119.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1100	UDP	O3'-C3'-C2'	-4.76	96.42	111.82
3	C	1101	UDP	O3'-C3'-C4'	-4.70	97.46	111.05
3	A	1100	UDP	C4-N3-C2	-4.39	120.79	126.58
3	C	1101	UDP	O2-C2-N3	-4.16	113.75	121.50
3	C	1101	UDP	C5-C6-N1	-4.15	114.86	121.81
4	B	101	9C1	C1-O5-C5	4.04	117.66	112.19
3	A	1100	UDP	N3-C2-N1	4.01	120.21	114.89
3	C	1101	UDP	PA-O3A-PB	-3.85	119.60	132.83
5	C	1102	9CD	C1-C2-N2	3.85	117.06	110.49
4	B	101	9C1	O3-C3-C2	-3.66	101.90	109.47
3	A	1100	UDP	C5-C4-N3	3.53	120.12	114.84
3	A	1100	UDP	O2'-C2'-C3'	-3.40	100.81	111.82
3	C	1101	UDP	O3B-PB-O3A	3.30	115.71	104.64
5	C	1102	9CD	O5-C5-C6	3.00	111.91	107.20
3	C	1101	UDP	O4'-C4'-C5'	2.92	119.00	109.37
3	C	1101	UDP	C2'-C3'-C4'	2.89	108.25	102.64
4	B	101	9C1	O14-C09-N2	-2.88	118.55	122.35
4	B	101	9C1	O14-C09-C10	-2.78	116.69	123.03
4	B	101	9C1	C1-C2-N2	-2.69	105.89	110.49
4	B	101	9C1	O3-C3-C4	-2.66	104.20	110.35
3	A	1100	UDP	PA-O3A-PB	-2.54	124.12	132.83
3	C	1101	UDP	O2B-PB-O3A	-2.50	96.25	104.64
4	B	101	9C1	C3-C4-C5	-2.50	105.79	110.24
3	A	1100	UDP	O4'-C1'-N1	-2.49	102.68	108.36
3	C	1101	UDP	C2'-C1'-N1	2.48	120.25	113.22
3	A	1100	UDP	O2-C2-N1	-2.41	119.58	122.79
3	A	1100	UDP	C2'-C1'-N1	2.39	119.99	113.22
3	C	1101	UDP	C4'-O4'-C1'	2.36	114.69	109.47
3	C	1101	UDP	C6-C5-C4	2.35	122.72	119.52
4	B	101	9C1	C6-C5-C4	-2.34	107.52	113.00
5	C	1102	9CD	O5-C5-C4	-2.30	105.24	110.83
3	C	1101	UDP	O3'-C3'-C2'	-2.27	104.49	111.82
3	A	1100	UDP	C2'-C3'-C4'	2.25	107.02	102.64
3	C	1101	UDP	O3B-PB-O2B	2.25	116.23	107.64
3	C	1101	UDP	O5'-C5'-C4'	-2.13	101.65	108.99
4	B	101	9C1	O4-C4-C5	-2.03	104.27	109.30

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1100	UDP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1101	UDP	C5'-O5'-PA-O1A
5	C	1102	9CD	O16-C12-C13-C14
5	C	1102	9CD	N2-C12-C13-C14
4	B	101	9C1	O5-C5-C6-O6
5	C	1102	9CD	O5-C5-C6-O6
5	C	1102	9CD	C4-C5-C6-O6
3	A	1100	UDP	O4'-C4'-C5'-O5'
3	A	1100	UDP	C3'-C4'-C5'-O5'
3	A	1100	UDP	PA-O3A-PB-O2B
3	C	1101	UDP	O4'-C4'-C5'-O5'

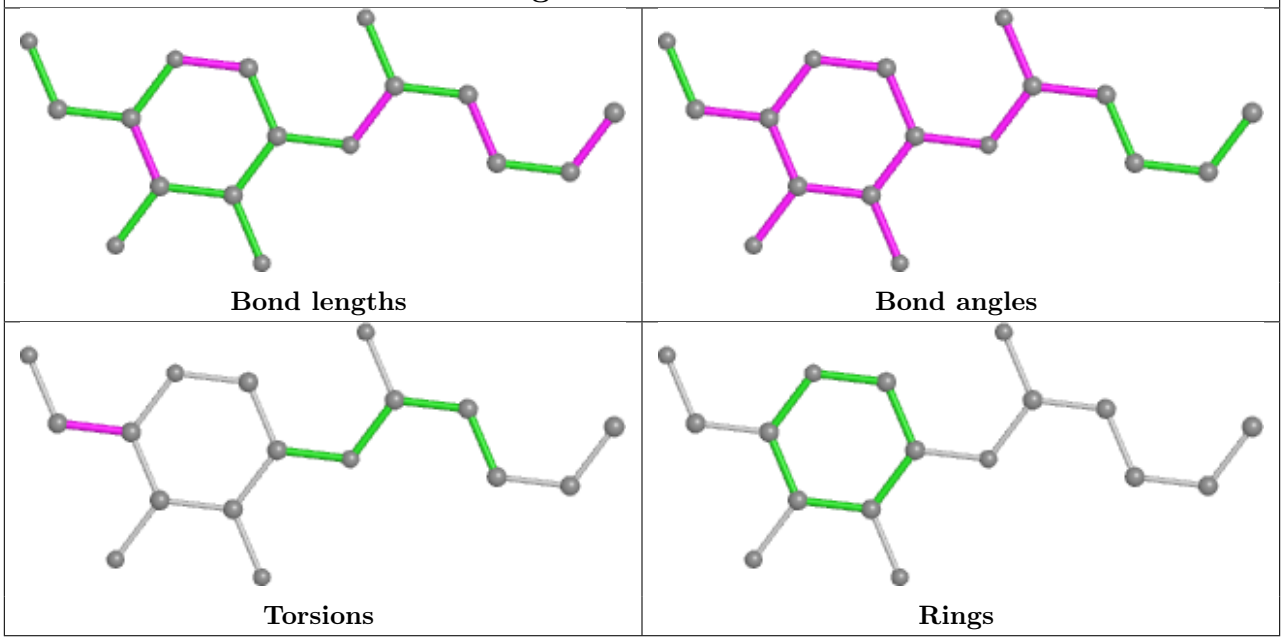
There are no ring outliers.

3 monomers are involved in 6 short contacts:

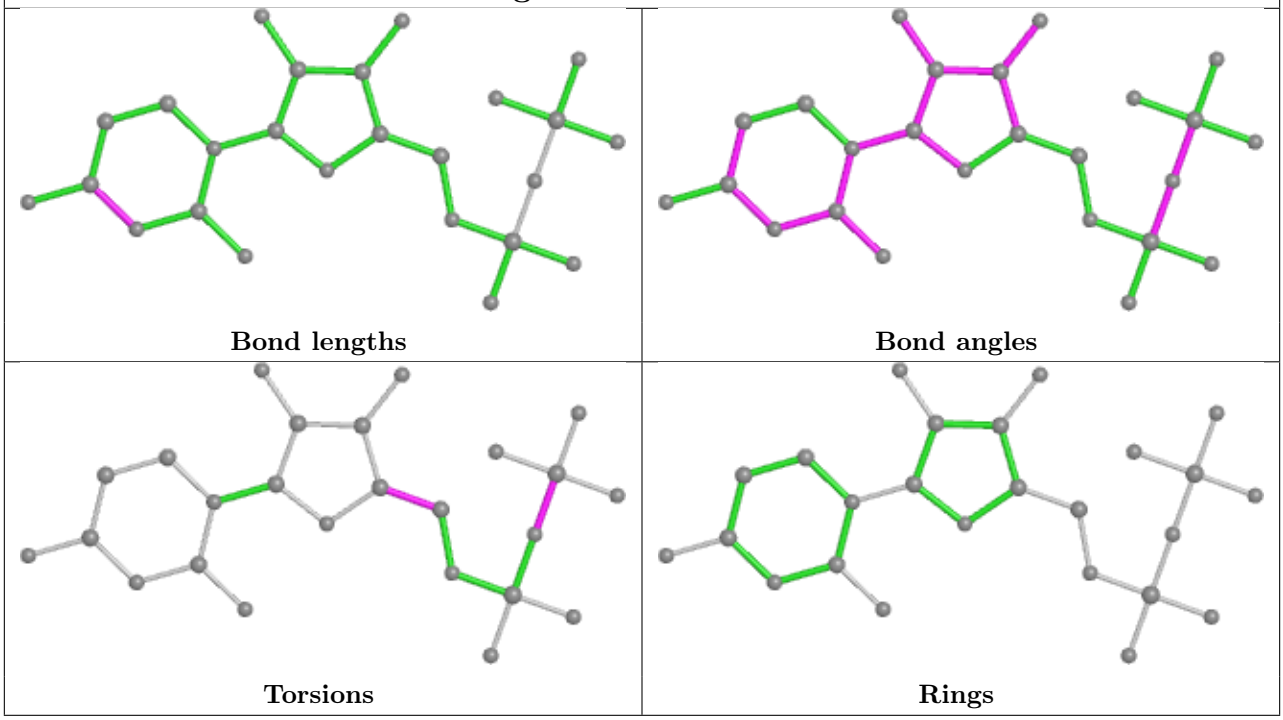
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	101	9C1	2	0
3	A	1100	UDP	2	0
3	C	1101	UDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

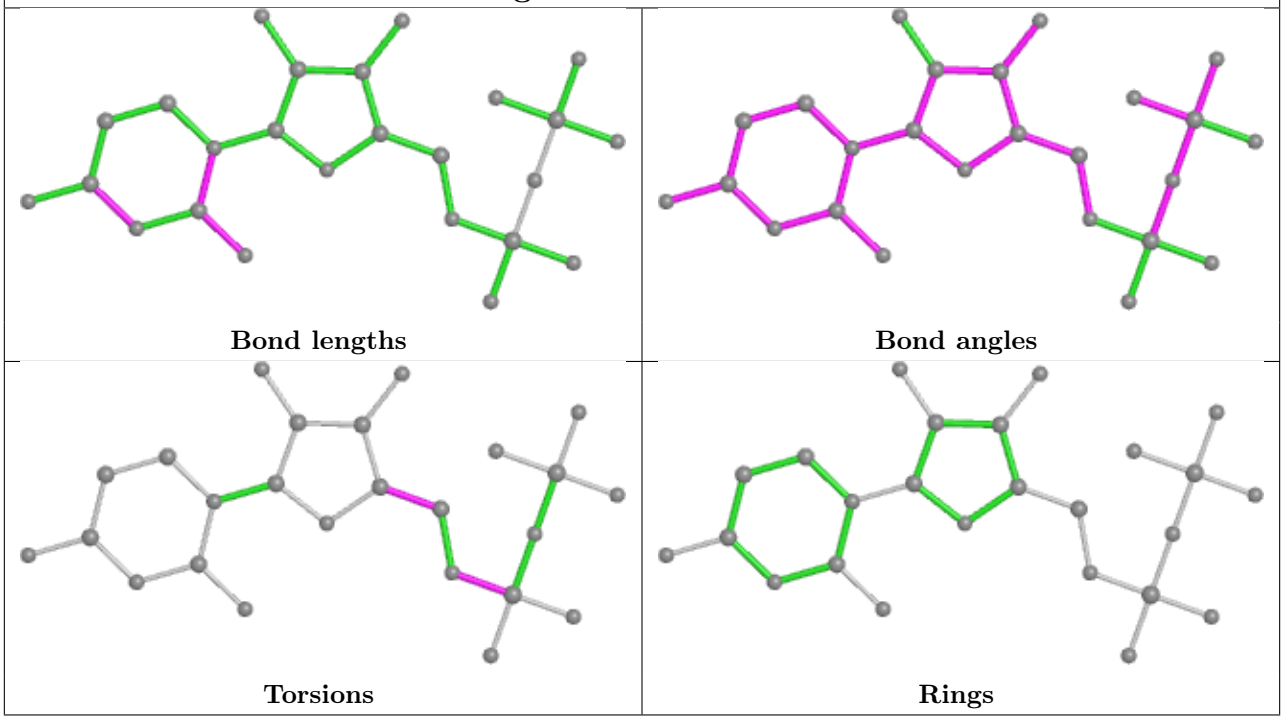
Ligand 9C1 B 101



Ligand UDP A 1100



Ligand UDP C 1101



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	666/723 (92%)	-0.07	17 (2%)	56	50	14, 39, 78, 124	0
1	C	667/723 (92%)	-0.11	11 (1%)	72	68	12, 38, 71, 106	0
2	B	12/14 (85%)	-0.27	0	100	100	23, 29, 32, 32	0
2	D	12/14 (85%)	-0.46	0	100	100	21, 30, 33, 35	0
All	All	1357/1474 (92%)	-0.09	28 (2%)	63	58	12, 38, 75, 124	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	PHE	3.6
1	C	346	VAL	3.5
1	A	345	GLU	3.2
1	C	528	LEU	3.1
1	C	345	GLU	3.1
1	C	343	ALA	3.1
1	A	347	PHE	3.0
1	C	342	LYS	3.0
1	C	353	ALA	2.7
1	A	363	GLN	2.7
1	A	740	ASP	2.7
1	C	678	VAL	2.7
1	A	342	LYS	2.6
1	A	527	VAL	2.5
1	A	769	MET	2.5
1	C	339	LEU	2.5
1	A	739	PRO	2.5
1	C	740	ASP	2.4
1	A	348	PRO	2.4
1	A	772	ILE	2.3
1	A	528	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	338	ARG	2.3
1	A	887	GLN	2.2
1	A	620	GLN	2.2
1	A	447	LYS	2.2
1	A	346	VAL	2.1
1	A	344	LEU	2.1
1	A	534	GLU	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

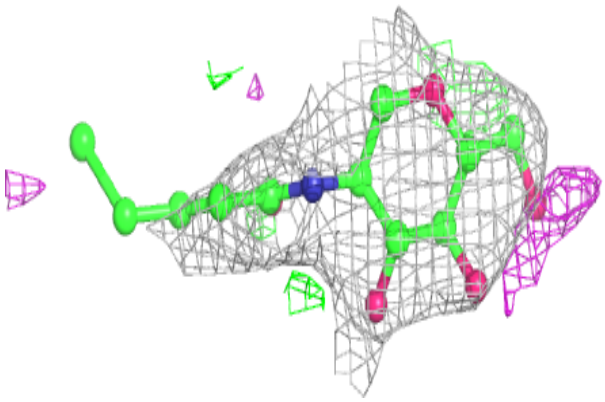
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

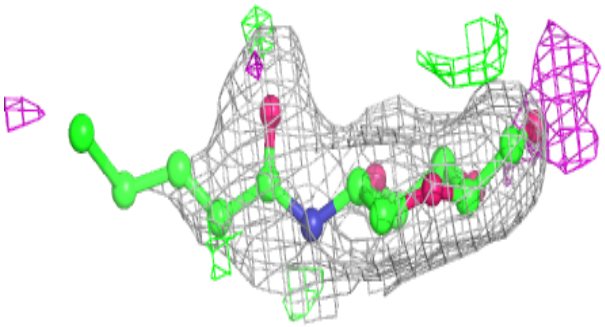
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	9C1	B	101	17/18	0.90	0.26	36,39,83,113	0
5	9CD	C	1102	16/17	0.93	0.17	30,38,41,43	0
3	UDP	A	1100	25/25	0.97	0.15	9,16,26,28	0
3	UDP	C	1101	25/25	0.97	0.17	9,16,26,26	0

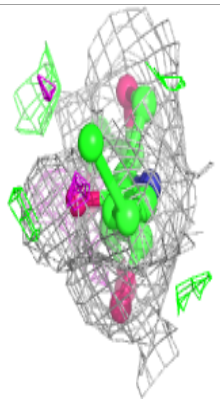
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 9C1 B 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

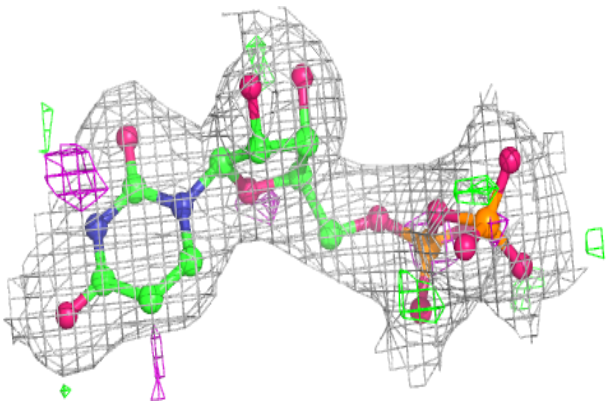


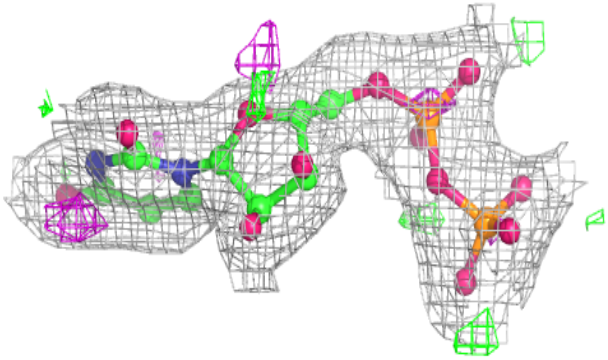


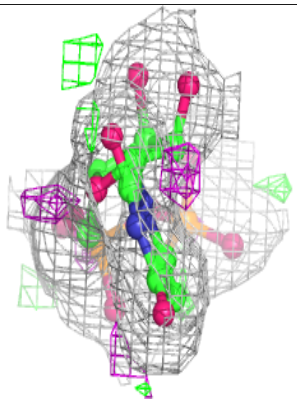


Electron density around UDP A 1100:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

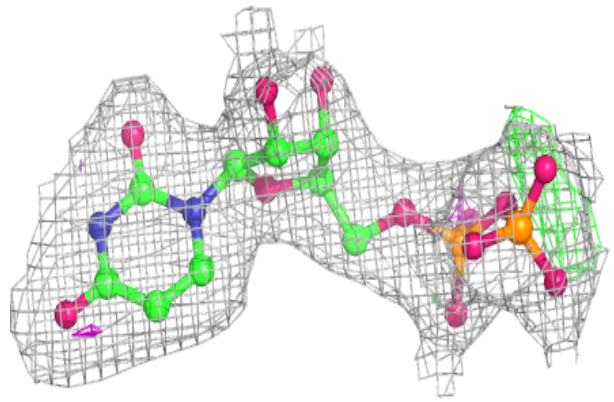


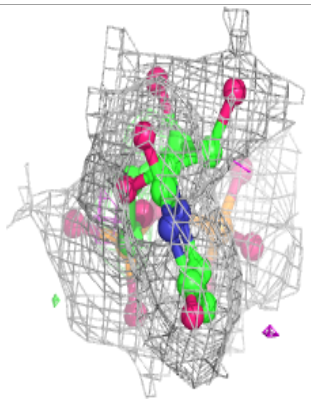




Electron density around UDP C 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.