



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:20 am BST

PDB ID : 5A01
Title : O-GlcNAc transferase from *Drosophila melanogaster*
Authors : Mariappa, D.; Zheng, X.; Schimpl, M.; Raimi, O.; Rafie, K.; Ferenbach, A.T.;
Mueller, H.J.; van Aalten, D.M.F.
Deposited on : 2015-04-15
Resolution : 2.66 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

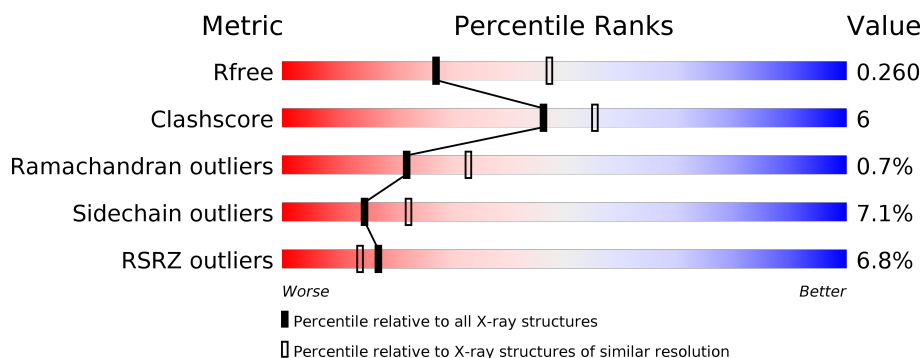
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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 $\leq 5\%$. 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	710	
1	B	710	
1	C	710	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16201 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.

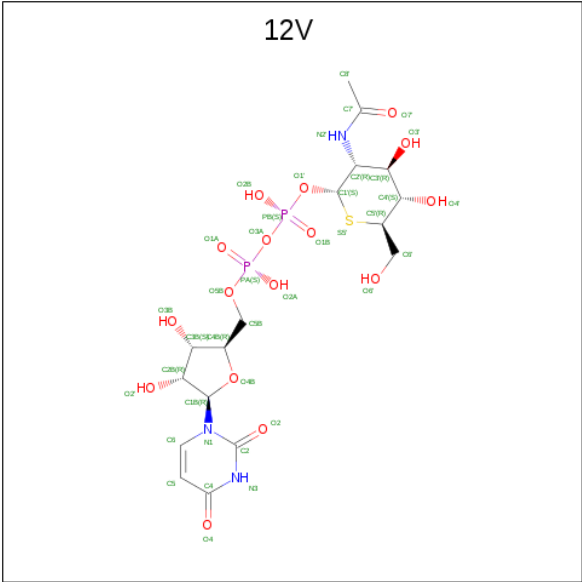
- Molecule 1 is a protein called O-GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	0	0	0
			5342	3393	930	989	30			
1	B	681	Total	C	N	O	S	0	0	0
			5342	3393	930	989	30			
1	C	681	Total	C	N	O	S	0	0	0
			5342	3393	930	989	30			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	GLY	-	expression tag	UNP Q7KJA9
A	351	PRO	-	expression tag	UNP Q7KJA9
A	872	MET	LYS	engineered mutation	UNP Q7KJA9
B	350	GLY	-	expression tag	UNP Q7KJA9
B	351	PRO	-	expression tag	UNP Q7KJA9
B	872	MET	LYS	engineered mutation	UNP Q7KJA9
C	350	GLY	-	expression tag	UNP Q7KJA9
C	351	PRO	-	expression tag	UNP Q7KJA9
C	872	MET	LYS	engineered mutation	UNP Q7KJA9

- Molecule 2 is (2S,3R,4R,5S,6R)-3-(acetylamino)-4,5-dihydroxy-6-(hydroxymethyl)tetrahydro-2H-thiopyran-2-yl [(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl dihydrogen diphosphate (three-letter code: 12V) (formula: C₁₇H₂₇N₃O₁₆P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

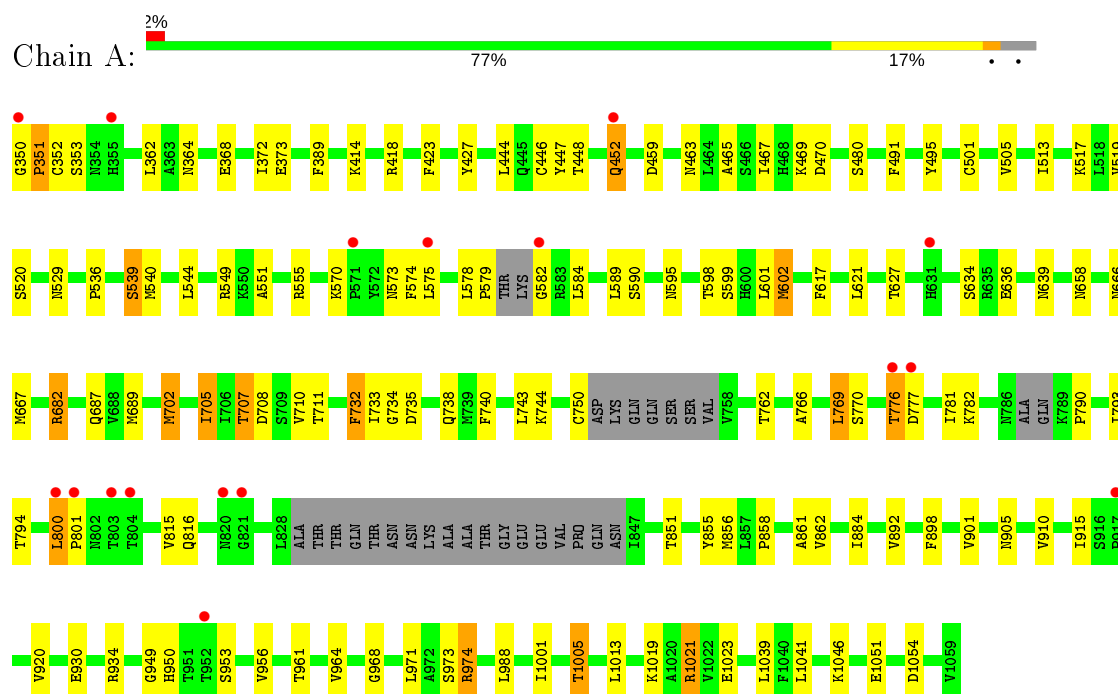
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	19	Total	O	0	0
			19	19		
3	C	6	Total	O	0	0
			6	6		

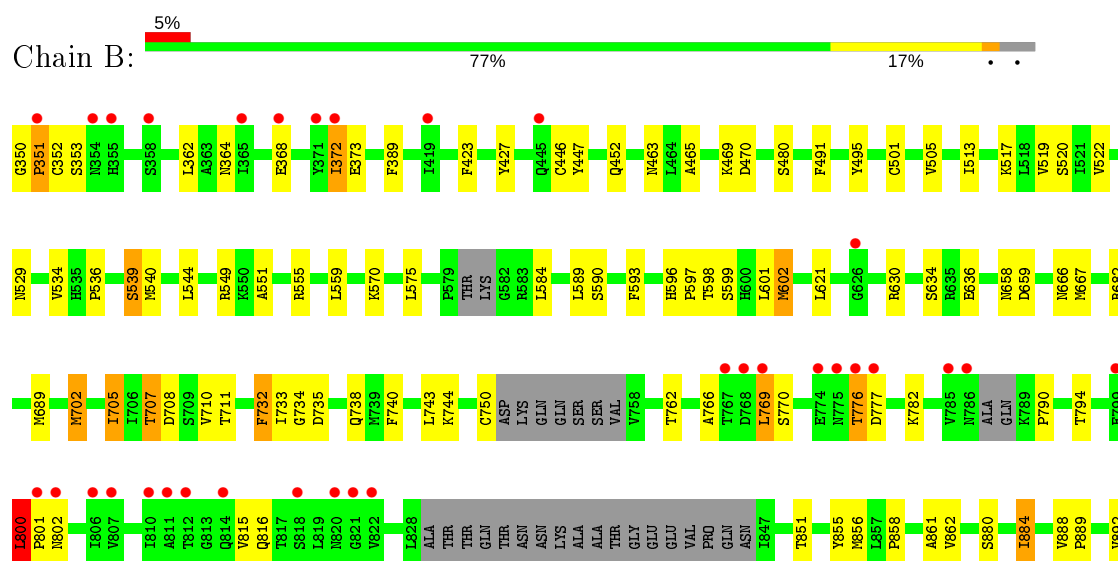
3 Residue-property plots [i](#)

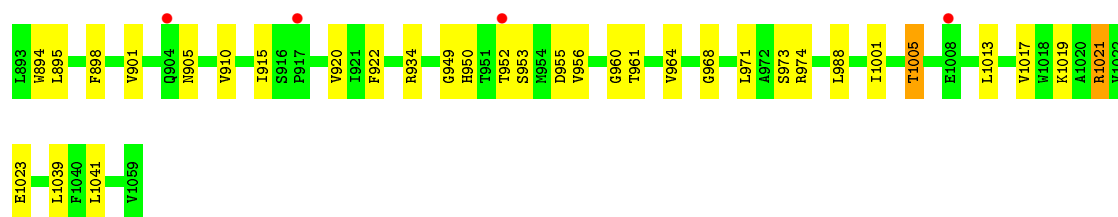
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($RSRZ > 2$). 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: O-GLYCOSYLTRANSFERASE

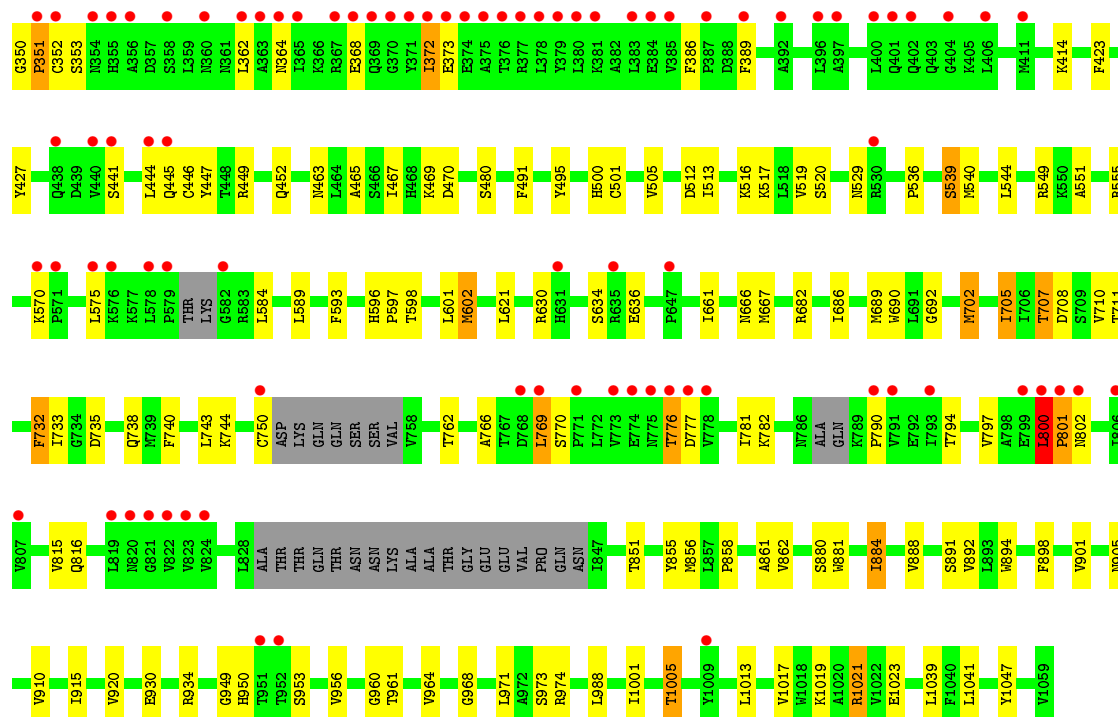
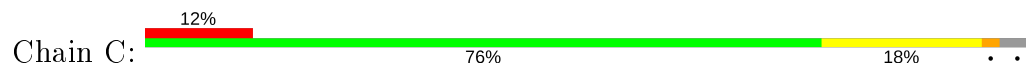


• Molecule 1: O-GLYCOSYLTRANSFERASE





● Molecule 1: O-GLYCOSYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	160.95Å 160.95Å 77.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.66 34.85 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.00-2.66) 99.7 (34.85-2.66)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.225 , 0.264 0.223 , 0.260	Depositor DCC
R_{free} test set	3237 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.037 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16201	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 41.83 % 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 2.2278e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 12V

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	0.54	0/5458	0.63	0/7410
1	B	0.53	1/5458 (0.0%)	0.62	0/7410
1	C	0.50	3/5458 (0.1%)	0.59	0/7410
All	All	0.52	4/16374 (0.0%)	0.61	0/22230

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	690	TRP	CD2-CE2	5.59	1.48	1.41
1	C	894	TRP	CD2-CE2	5.09	1.47	1.41
1	B	894	TRP	CD2-CE2	5.02	1.47	1.41
1	C	881	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	PHE	Peptide

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	5342	0	5302	76	0
1	B	5342	0	5302	63	0
1	C	5342	0	5302	78	0
2	A	39	0	25	1	0
2	B	39	0	25	1	0
2	C	39	0	25	1	0
3	A	33	0	0	0	0
3	B	19	0	0	0	0
3	C	6	0	0	0	0
All	All	16201	0	15981	201	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 6.

All (201) 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:C:351:PRO:HA	1:C:353:SER:H	1.23	1.03
1:B:351:PRO:HA	1:B:353:SER:H	1.25	1.00
1:A:579:PRO:HD3	1:C:445:GLN:HE21	1.29	0.98
1:A:351:PRO:HA	1:A:353:SER:H	1.26	0.96
1:C:351:PRO:HA	1:C:353:SER:N	1.80	0.95
1:B:351:PRO:HA	1:B:353:SER:N	1.82	0.94
1:A:579:PRO:HB2	1:C:441:SER:OG	1.66	0.94
1:A:351:PRO:HA	1:A:353:SER:N	1.83	0.92
1:A:579:PRO:HD3	1:C:445:GLN:NE2	1.86	0.91
1:A:418:ARG:HB2	1:B:658:ASN:OD1	1.75	0.87
1:B:782:LYS:HE2	1:B:794:THR:HG22	1.58	0.86
1:C:782:LYS:HE2	1:C:794:THR:HG22	1.57	0.85
1:A:782:LYS:HE2	1:A:794:THR:HG22	1.59	0.82
1:A:579:PRO:CB	1:C:441:SER:OG	2.31	0.79
1:C:539:SER:HB3	1:C:549:ARG:HD3	1.67	0.75
1:C:762:THR:HG23	1:C:851:THR:HG22	1.71	0.71
1:A:582:GLY:N	1:C:441:SER:HG	1.89	0.70
1:A:950:HIS:HD2	2:A:2060:12V:O3'	1.75	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:950:HIS:HD2	2:C:2060:12V:O3'	1.75	0.69
1:A:536:PRO:O	1:A:539:SER:HB2	1.94	0.68
1:B:539:SER:HB3	1:B:549:ARG:HD3	1.75	0.67
1:B:762:THR:HG23	1:B:851:THR:HG22	1.75	0.67
1:A:762:THR:HG23	1:A:851:THR:HG22	1.78	0.66
1:B:782:LYS:HE2	1:B:794:THR:CG2	2.26	0.66
1:A:658:ASN:O	1:C:414:LYS:HD3	1.96	0.64
1:C:782:LYS:HE2	1:C:794:THR:CG2	2.27	0.63
1:A:782:LYS:HE2	1:A:794:THR:CG2	2.27	0.63
1:B:536:PRO:O	1:B:539:SER:HB2	1.98	0.63
1:C:732:PHE:CZ	1:C:950:HIS:HB3	2.34	0.62
1:C:364:ASN:O	1:C:368:GLU:HG2	2.00	0.62
1:A:469:LYS:HD2	1:A:501:CYS:SG	2.40	0.61
1:A:732:PHE:CZ	1:A:950:HIS:HB3	2.35	0.61
1:A:579:PRO:CG	1:C:441:SER:OG	2.48	0.61
1:B:732:PHE:CZ	1:B:950:HIS:HB3	2.35	0.61
1:C:740:PHE:HB3	1:C:743:LEU:HD12	1.83	0.61
1:A:949:GLY:O	1:A:953:SER:HB3	2.01	0.61
1:B:519:VAL:HG22	1:B:544:LEU:HD23	1.83	0.61
1:C:815:VAL:HG12	1:C:816:GLN:HG3	1.83	0.60
1:A:519:VAL:HG22	1:A:544:LEU:HD23	1.82	0.60
1:C:536:PRO:O	1:C:539:SER:HB2	2.02	0.60
1:A:539:SER:HB3	1:A:549:ARG:HD3	1.84	0.60
1:B:968:GLY:H	1:B:973:SER:HB3	1.68	0.59
1:A:350:GLY:O	1:A:352:CYS:HB3	2.03	0.59
1:A:589:LEU:HD21	1:A:621:LEU:HD11	1.84	0.58
1:A:968:GLY:H	1:A:973:SER:HB3	1.69	0.58
1:B:1019:LYS:HE3	1:B:1023:GLU:OE2	2.04	0.58
1:B:950:HIS:HD2	2:B:2060:12V:O3'	1.86	0.58
1:C:519:VAL:HG22	1:C:544:LEU:HD23	1.85	0.58
1:B:689:MET:HB2	1:B:705:ILE:HG12	1.86	0.57
1:B:740:PHE:HB3	1:B:743:LEU:HD12	1.87	0.57
1:C:689:MET:HB2	1:C:705:ILE:HG12	1.87	0.56
1:C:350:GLY:O	1:C:352:CYS:HB3	2.05	0.56
1:B:364:ASN:O	1:B:368:GLU:HG2	2.05	0.56
1:B:815:VAL:HG12	1:B:816:GLN:HG3	1.86	0.56
1:B:949:GLY:O	1:B:953:SER:HB3	2.05	0.56
1:C:469:LYS:HD2	1:C:501:CYS:SG	2.45	0.56
1:C:949:GLY:O	1:C:953:SER:HB3	2.05	0.56
1:A:740:PHE:HB3	1:A:743:LEU:HD12	1.88	0.56
1:B:350:GLY:O	1:B:352:CYS:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:VAL:O	1:C:974:ARG:NH1	2.39	0.56
1:A:1019:LYS:HE3	1:A:1023:GLU:OE2	2.07	0.55
1:A:689:MET:HB2	1:A:705:ILE:HG12	1.88	0.55
1:A:815:VAL:HG12	1:A:816:GLN:HG3	1.88	0.55
1:C:1019:LYS:HE3	1:C:1023:GLU:OE2	2.07	0.55
1:C:968:GLY:H	1:C:973:SER:HB3	1.72	0.55
1:B:469:LYS:HD2	1:B:501:CYS:SG	2.47	0.54
1:A:658:ASN:O	1:C:414:LYS:CE	2.55	0.54
1:B:988:LEU:HD21	1:B:1013:LEU:HD21	1.88	0.54
1:B:858:PRO:HB2	1:B:861:ALA:HB2	1.89	0.53
1:A:858:PRO:HB2	1:A:861:ALA:HB2	1.90	0.53
1:A:579:PRO:HG2	1:C:441:SER:O	2.09	0.53
1:C:598:THR:HG22	1:C:602:MET:HE2	1.90	0.52
1:A:599:SER:HA	1:A:602:MET:HE3	1.91	0.52
1:A:364:ASN:O	1:A:368:GLU:HG2	2.09	0.52
1:C:495:TYR:CZ	1:C:517:LYS:HD3	2.44	0.52
1:B:551:ALA:O	1:B:555:ARG:HG3	2.09	0.52
1:A:1001:ILE:O	1:A:1005:THR:HB	2.10	0.52
1:B:855:TYR:CE1	1:B:934:ARG:HD3	2.45	0.51
1:A:988:LEU:HD21	1:A:1013:LEU:HD21	1.93	0.50
1:C:551:ALA:O	1:C:555:ARG:HG3	2.10	0.50
1:A:505:VAL:HG12	1:A:905:ASN:ND2	2.27	0.50
1:A:589:LEU:CD2	1:A:621:LEU:HD11	2.41	0.50
1:A:710:VAL:O	1:A:974:ARG:NH1	2.44	0.50
1:B:952:THR:HA	1:B:955:ASP:OD2	2.13	0.49
1:B:710:VAL:O	1:B:974:ARG:NH1	2.45	0.49
1:C:1001:ILE:O	1:C:1005:THR:HB	2.12	0.49
1:C:735:ASP:OD1	1:C:738:GLN:NE2	2.32	0.48
1:B:447:TYR:CZ	1:B:463:ASN:HB3	2.48	0.48
1:A:658:ASN:O	1:C:414:LYS:CD	2.62	0.48
1:C:910:VAL:HG21	1:C:920:VAL:HG21	1.96	0.48
1:A:427:TYR:O	1:A:446:CYS:HB3	2.13	0.48
1:B:1001:ILE:O	1:B:1005:THR:HB	2.14	0.48
1:C:667:MET:O	1:C:692:GLY:HA3	2.13	0.48
1:C:766:ALA:HB3	1:C:769:LEU:HD23	1.96	0.48
1:A:930:GLU:O	1:A:934:ARG:HG3	2.13	0.47
1:C:505:VAL:HG12	1:C:505:VAL:O	2.14	0.47
1:B:593:PHE:O	1:B:630:ARG:HD3	2.14	0.47
1:A:495:TYR:CZ	1:A:517:LYS:HD3	2.50	0.47
1:C:465:ALA:HB2	1:C:480:SER:CB	2.45	0.47
1:C:988:LEU:HD21	1:C:1013:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ALA:O	1:A:555:ARG:HG3	2.15	0.46
1:B:711:THR:HG22	1:B:971:LEU:HG	1.97	0.46
1:A:735:ASP:OD1	1:A:738:GLN:NE2	2.40	0.46
1:B:598:THR:HG22	1:B:602:MET:HE2	1.96	0.46
1:A:573:ASN:ND2	1:C:449:ARG:NH2	2.63	0.46
1:B:956:VAL:HG13	1:B:961:THR:HB	1.98	0.46
1:A:447:TYR:CZ	1:A:463:ASN:HB3	2.50	0.46
1:B:465:ALA:HB2	1:B:480:SER:CB	2.46	0.46
1:B:910:VAL:HG21	1:B:920:VAL:HG21	1.98	0.46
1:A:956:VAL:CG1	1:A:961:THR:HB	2.46	0.46
1:B:744:LYS:HA	1:B:1021:ARG:HH22	1.81	0.46
1:B:666:ASN:HB2	1:B:702:MET:HE1	1.98	0.45
1:A:448:THR:O	1:A:452:GLN:HG3	2.17	0.45
1:A:711:THR:HG22	1:A:971:LEU:HG	1.98	0.45
1:B:590:SER:HB2	1:B:667:MET:HB2	1.99	0.45
1:A:579:PRO:HD2	1:C:441:SER:OG	2.17	0.45
1:C:589:LEU:HD21	1:C:621:LEU:HD11	1.98	0.45
1:C:469:LYS:NZ	1:C:500:HIS:ND1	2.62	0.45
1:A:855:TYR:CE1	1:A:934:ARG:HD3	2.52	0.45
1:C:956:VAL:HG13	1:C:961:THR:HB	1.99	0.45
1:A:766:ALA:HB3	1:A:769:LEU:HD23	1.98	0.45
1:A:915:ILE:HA	1:A:915:ILE:HD13	1.86	0.45
1:B:895:LEU:O	1:B:922:PHE:HA	2.15	0.45
1:C:744:LYS:HA	1:C:1021:ARG:HH22	1.81	0.45
1:B:915:ILE:HA	1:B:915:ILE:HD13	1.90	0.45
1:A:666:ASN:HB2	1:A:702:MET:HE1	1.99	0.44
1:B:495:TYR:CZ	1:B:517:LYS:HD3	2.51	0.44
1:B:505:VAL:HG12	1:B:905:ASN:ND2	2.32	0.44
1:B:465:ALA:HB2	1:B:480:SER:HB3	1.99	0.44
1:B:956:VAL:CG1	1:B:961:THR:HB	2.47	0.44
1:A:956:VAL:HG13	1:A:961:THR:HB	1.98	0.44
1:B:427:TYR:O	1:B:446:CYS:HB3	2.17	0.44
1:B:707:THR:HB	1:B:708:ASP:H	1.32	0.44
1:A:598:THR:HG22	1:A:602:MET:HE2	2.00	0.44
1:B:766:ALA:HB3	1:B:769:LEU:HD23	1.99	0.44
1:B:597:PRO:O	1:B:601:LEU:HG	2.18	0.44
1:C:447:TYR:CZ	1:C:463:ASN:HB3	2.52	0.44
1:B:596:HIS:CG	1:B:597:PRO:HD2	2.53	0.44
1:C:444:LEU:HD13	1:C:467:ILE:HG21	2.00	0.43
1:A:465:ALA:HB2	1:A:480:SER:CB	2.49	0.43
1:A:505:VAL:HG12	1:A:505:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:SER:HB2	1:A:667:MET:HB2	2.01	0.43
1:A:579:PRO:CD	1:C:441:SER:OG	2.66	0.43
1:C:597:PRO:O	1:C:601:LEU:HG	2.18	0.43
1:C:855:TYR:CE1	1:C:934:ARG:HD3	2.53	0.43
1:A:444:LEU:HD13	1:A:467:ILE:HG21	2.01	0.43
1:B:735:ASP:OD1	1:B:738:GLN:NE2	2.40	0.43
1:C:686:ILE:HD11	1:C:1047:TYR:HB2	2.00	0.43
1:C:858:PRO:HB2	1:C:861:ALA:HB2	2.00	0.43
1:A:744:LYS:HA	1:A:1021:ARG:HH22	1.84	0.42
1:A:707:THR:HB	1:A:708:ASP:H	1.32	0.42
1:C:505:VAL:HG12	1:C:905:ASN:ND2	2.35	0.42
1:C:711:THR:HG22	1:C:971:LEU:HG	2.00	0.42
1:A:601:LEU:HA	1:A:734:GLY:HA2	2.02	0.42
1:B:880:SER:O	1:B:884:ILE:HG23	2.18	0.42
1:A:469:LYS:CD	1:A:501:CYS:SG	3.06	0.42
1:B:599:SER:HA	1:B:602:MET:HE3	2.02	0.42
1:A:1046:LYS:NZ	1:A:1054:ASP:HB3	2.35	0.42
1:C:776:THR:HG22	1:C:777:ASP:H	1.85	0.42
1:A:910:VAL:HG21	1:A:920:VAL:HG21	2.00	0.42
1:C:598:THR:O	1:C:602:MET:HE3	2.20	0.42
1:A:617:PHE:HA	1:A:639:ASN:HB2	2.01	0.42
1:B:776:THR:HG22	1:B:777:ASP:H	1.84	0.42
1:C:372:ILE:HG13	1:C:372:ILE:H	1.68	0.42
1:C:427:TYR:O	1:C:446:CYS:HB3	2.19	0.42
1:C:915:ILE:HA	1:C:915:ILE:HD13	1.95	0.42
1:C:800:LEU:N	1:C:801:PRO:CD	2.83	0.42
1:C:512:ASP:O	1:C:516:LYS:HG2	2.20	0.41
1:C:666:ASN:HB2	1:C:702:MET:HE1	2.00	0.41
1:C:781:ILE:HG22	1:C:782:LYS:N	2.35	0.41
1:C:353:SER:HB3	1:C:386:PHE:CE2	2.55	0.41
1:C:596:HIS:CG	1:C:597:PRO:HD2	2.55	0.41
1:C:956:VAL:CG1	1:C:961:THR:HB	2.50	0.41
1:C:960:GLY:HA2	1:C:1017:VAL:HG12	2.02	0.41
1:A:1019:LYS:HA	1:A:1019:LYS:HD2	1.83	0.41
1:B:559:LEU:HA	1:B:559:LEU:HD23	1.94	0.41
1:A:448:THR:O	1:A:452:GLN:CG	2.68	0.41
1:C:593:PHE:O	1:C:630:ARG:HD3	2.20	0.41
1:B:505:VAL:O	1:B:505:VAL:HG12	2.20	0.41
1:C:707:THR:HB	1:C:708:ASP:H	1.45	0.41
1:C:880:SER:O	1:C:884:ILE:HG23	2.21	0.41
1:A:682:ARG:NH1	1:A:687:GLN:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:LEU:HD21	1:B:621:LEU:HD11	2.02	0.41
1:C:1019:LYS:HA	1:C:1019:LYS:HD2	1.83	0.41
1:B:800:LEU:O	1:B:802:ASN:N	2.53	0.41
1:C:930:GLU:O	1:C:934:ARG:HG3	2.20	0.41
1:A:781:ILE:HG22	1:A:782:LYS:N	2.35	0.41
1:B:522:VAL:HG21	1:B:534:VAL:HG11	2.03	0.41
1:A:414:LYS:NZ	1:B:659:ASP:HA	2.36	0.41
1:A:578:LEU:HA	1:C:445:GLN:NE2	2.35	0.41
1:A:595:ASN:HB2	1:A:627:THR:HG21	2.03	0.41
1:B:888:VAL:HA	1:B:889:PRO:HD3	1.94	0.41
1:C:888:VAL:HG12	1:C:891:SER:HB3	2.02	0.41
1:B:372:ILE:H	1:B:372:ILE:HG13	1.62	0.40
1:B:601:LEU:HA	1:B:734:GLY:HA2	2.03	0.40
1:B:960:GLY:HA2	1:B:1017:VAL:HG12	2.03	0.40
1:C:781:ILE:HD12	1:C:797:VAL:HG21	2.02	0.40
1:A:776:THR:HG22	1:A:777:ASP:H	1.86	0.40
1:C:800:LEU:O	1:C:802:ASN:N	2.55	0.40
1:A:1046:LYS:O	1:A:1051:GLU:HB2	2.21	0.40
1:B:658:ASN:HA	1:B:658:ASN:HD22	1.71	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	671/710 (94%)	650 (97%)	16 (2%)	5 (1%)	22	33
1	B	671/710 (94%)	648 (97%)	18 (3%)	5 (1%)	22	33
1	C	671/710 (94%)	649 (97%)	17 (2%)	5 (1%)	22	33
All	All	2013/2130 (94%)	1947 (97%)	51 (2%)	15 (1%)	22	33

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	790	PRO
1	A	801	PRO
1	B	790	PRO
1	B	801	PRO
1	C	790	PRO
1	C	801	PRO
1	A	539	SER
1	B	539	SER
1	C	539	SER
1	A	351	PRO
1	A	800	LEU
1	B	351	PRO
1	B	800	LEU
1	C	351	PRO
1	C	800	LEU

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	583/620 (94%)	540 (93%)	43 (7%)	13	21
1	B	583/620 (94%)	543 (93%)	40 (7%)	15	24
1	C	583/620 (94%)	542 (93%)	41 (7%)	15	23
All	All	1749/1860 (94%)	1625 (93%)	124 (7%)	14	22

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	LEU
1	A	372	ILE
1	A	373	GLU
1	A	389	PHE
1	A	423	PHE
1	A	452	GLN
1	A	459	ASP
1	A	470	ASP

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Mol	Chain	Res	Type
1	A	491	PHE
1	A	513	ILE
1	A	520	SER
1	A	529	ASN
1	A	540	MET
1	A	570	LYS
1	A	575	LEU
1	A	584	LEU
1	A	602	MET
1	A	634	SER
1	A	636	GLU
1	A	682	ARG
1	A	702	MET
1	A	705	ILE
1	A	707	THR
1	A	732	PHE
1	A	733	ILE
1	A	750	CYS
1	A	769	LEU
1	A	770	SER
1	A	776	THR
1	A	793	ILE
1	A	800	LEU
1	A	856	MET
1	A	862	VAL
1	A	884	ILE
1	A	892	VAL
1	A	898	PHE
1	A	901	VAL
1	A	964	VAL
1	A	974	ARG
1	A	1005	THR
1	A	1021	ARG
1	A	1039	LEU
1	A	1041	LEU
1	B	362	LEU
1	B	372	ILE
1	B	373	GLU
1	B	389	PHE
1	B	423	PHE
1	B	452	GLN
1	B	470	ASP

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Mol	Chain	Res	Type
1	B	491	PHE
1	B	513	ILE
1	B	520	SER
1	B	529	ASN
1	B	540	MET
1	B	570	LYS
1	B	575	LEU
1	B	584	LEU
1	B	602	MET
1	B	634	SER
1	B	636	GLU
1	B	682	ARG
1	B	702	MET
1	B	705	ILE
1	B	707	THR
1	B	732	PHE
1	B	733	ILE
1	B	750	CYS
1	B	769	LEU
1	B	770	SER
1	B	776	THR
1	B	800	LEU
1	B	856	MET
1	B	862	VAL
1	B	884	ILE
1	B	892	VAL
1	B	898	PHE
1	B	901	VAL
1	B	964	VAL
1	B	1005	THR
1	B	1021	ARG
1	B	1039	LEU
1	B	1041	LEU
1	C	362	LEU
1	C	372	ILE
1	C	373	GLU
1	C	389	PHE
1	C	423	PHE
1	C	452	GLN
1	C	470	ASP
1	C	491	PHE
1	C	513	ILE

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Mol	Chain	Res	Type
1	C	520	SER
1	C	529	ASN
1	C	540	MET
1	C	570	LYS
1	C	575	LEU
1	C	584	LEU
1	C	602	MET
1	C	634	SER
1	C	636	GLU
1	C	661	ILE
1	C	682	ARG
1	C	702	MET
1	C	705	ILE
1	C	707	THR
1	C	732	PHE
1	C	733	ILE
1	C	750	CYS
1	C	769	LEU
1	C	770	SER
1	C	776	THR
1	C	800	LEU
1	C	856	MET
1	C	862	VAL
1	C	884	ILE
1	C	892	VAL
1	C	898	PHE
1	C	901	VAL
1	C	964	VAL
1	C	1005	THR
1	C	1021	ARG
1	C	1039	LEU
1	C	1041	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	503	GLN
1	A	573	ASN
1	A	658	ASN
1	A	869	GLN
1	A	950	HIS
1	A	1031	GLN

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Mol	Chain	Res	Type
1	B	503	GLN
1	B	869	GLN
1	B	950	HIS
1	B	1031	GLN
1	C	445	GLN
1	C	503	GLN
1	C	556	HIS
1	C	658	ASN
1	C	869	GLN
1	C	950	HIS
1	C	1031	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	12V	C	2060	-	32,41,41	1.40	4 (12%)	38,62,62	1.14	3 (7%)
2	12V	B	2060	-	32,41,41	1.78	5 (15%)	38,62,62	1.23	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	12V	A	2060	-	32,41,41	1.57	3 (9%)	38,62,62	1.18	4 (10%)

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	12V	C	2060	-	-	6/23/63/63	0/3/3/3
2	12V	B	2060	-	-	5/23/63/63	0/3/3/3
2	12V	A	2060	-	-	9/23/63/63	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2060	12V	C6-N1	5.18	1.42	1.35
2	B	2060	12V	C4-N3	4.61	1.41	1.33
2	A	2060	12V	C6-N1	4.20	1.41	1.35
2	C	2060	12V	C4-N3	4.19	1.40	1.33
2	C	2060	12V	C6-N1	4.05	1.40	1.35
2	A	2060	12V	C4-N3	4.01	1.40	1.33
2	A	2060	12V	C5'-S5'	-3.97	1.76	1.82
2	B	2060	12V	C4'-C5'	-3.76	1.50	1.53
2	B	2060	12V	C6'-C5'	3.02	1.54	1.52
2	B	2060	12V	O4B-C1B	2.55	1.44	1.41
2	C	2060	12V	PB-O1'	2.47	1.67	1.60
2	C	2060	12V	C5'-S5'	-2.41	1.78	1.82

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2060	12V	O4B-C1B-C2B	-4.22	100.76	106.93
2	C	2060	12V	O4B-C1B-C2B	-3.30	102.10	106.93
2	A	2060	12V	C4'-C3'-C2'	3.05	114.81	110.34
2	B	2060	12V	C5B-C4B-C3B	-2.81	104.64	115.18
2	B	2060	12V	C4'-C3'-C2'	2.55	114.08	110.34
2	A	2060	12V	PB-O3A-PA	-2.51	124.22	132.83
2	A	2060	12V	C3'-C2'-N2'	-2.48	105.93	110.62
2	C	2060	12V	PB-O3A-PA	-2.44	124.45	132.83
2	C	2060	12V	O1'-C1'-C2'	2.39	111.08	107.47
2	A	2060	12V	O4B-C1B-C2B	-2.33	103.52	106.93

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2060	12V	C3B-C4B-C5B-O5B
2	B	2060	12V	C5B-O5B-PA-O1A
2	B	2060	12V	C5B-O5B-PA-O3A
2	A	2060	12V	C2B-C1B-N1-C6
2	A	2060	12V	O4B-C1B-N1-C6
2	A	2060	12V	C5B-O5B-PA-O3A
2	A	2060	12V	C3B-C4B-C5B-O5B
2	C	2060	12V	O4B-C4B-C5B-O5B
2	A	2060	12V	O4B-C4B-C5B-O5B
2	A	2060	12V	C4'-C5'-C6'-O6'
2	C	2060	12V	C5B-O5B-PA-O3A
2	C	2060	12V	PA-O3A-PB-O2B
2	B	2060	12V	C5B-O5B-PA-O2A
2	A	2060	12V	C5B-O5B-PA-O1A
2	A	2060	12V	C5B-O5B-PA-O2A
2	B	2060	12V	PB-O3A-PA-O1A
2	C	2060	12V	PA-O3A-PB-O1B
2	B	2060	12V	PB-O3A-PA-O2A
2	A	2060	12V	PA-O3A-PB-O2B
2	C	2060	12V	C5B-O5B-PA-O1A

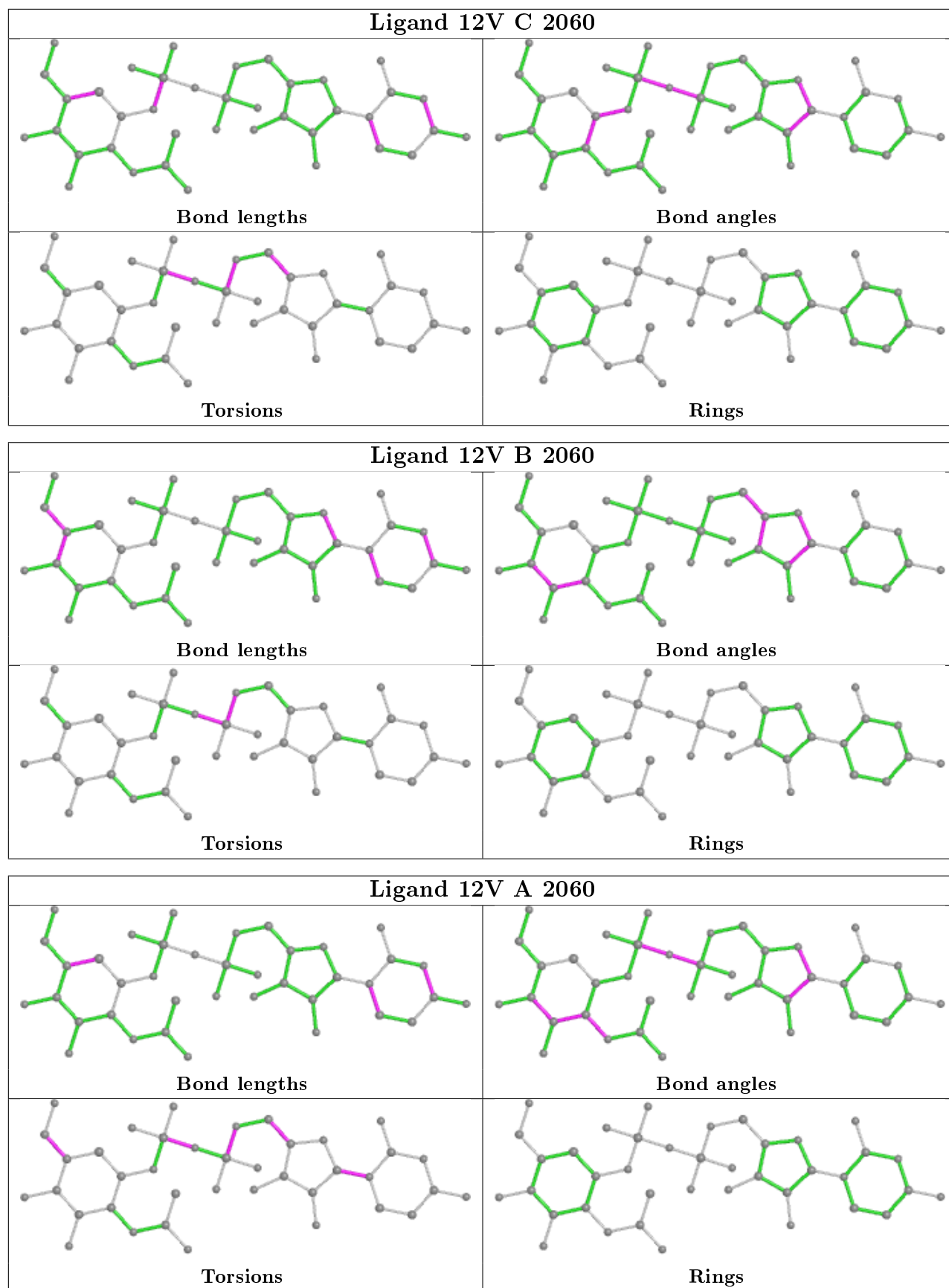
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2060	12V	1	0
2	B	2060	12V	1	0
2	A	2060	12V	1	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 than 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.



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

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	681/710 (95%)	0.12	17 (2%) 57 53	25, 40, 70, 116	8 (1%)
1	B	681/710 (95%)	0.20	37 (5%) 25 23	21, 44, 83, 119	8 (1%)
1	C	681/710 (95%)	0.62	84 (12%) 4 2	33, 55, 102, 139	8 (1%)
All	All	2043/2130 (95%)	0.31	138 (6%) 17 14	21, 46, 91, 139	24 (1%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	355	HIS	7.9
1	C	380	LEU	7.3
1	C	440	VAL	7.0
1	C	379	TYR	6.6
1	C	441	SER	6.4
1	C	383	LEU	6.3
1	C	578	LEU	6.2
1	C	377	ARG	5.9
1	C	376	THR	5.9
1	B	820	ASN	5.8
1	C	801	PRO	5.4
1	C	575	LEU	5.4
1	C	352	CYS	5.2
1	C	821	GLY	5.1
1	C	802	ASN	5.0
1	C	777	ASP	4.9
1	C	579	PRO	4.7
1	C	371	TYR	4.5
1	C	384	GLU	4.5
1	C	389	PHE	4.3
1	C	952	THR	4.3
1	B	768	ASP	4.3
1	C	375	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	370	GLY	4.3
1	B	777	ASP	4.0
1	C	768	ASP	4.0
1	A	801	PRO	3.8
1	C	367	ARG	3.8
1	C	576	LYS	3.8
1	B	786	ASN	3.8
1	C	582	GLY	3.7
1	C	358	SER	3.7
1	C	378	LEU	3.7
1	C	372	ILE	3.7
1	C	369	GLN	3.6
1	B	785	VAL	3.6
1	B	822	VAL	3.5
1	C	362	LEU	3.5
1	C	773	VAL	3.5
1	C	822	VAL	3.5
1	C	356	ALA	3.5
1	B	952	THR	3.4
1	C	774	GLU	3.4
1	C	401	GLN	3.4
1	B	812	THR	3.3
1	A	821	GLY	3.3
1	C	775	ASN	3.3
1	C	387	PRO	3.3
1	B	821	GLY	3.3
1	A	952	THR	3.3
1	C	381	LYS	3.3
1	C	368	GLU	3.2
1	A	917	PRO	3.2
1	C	397	ALA	3.2
1	B	811	ALA	3.2
1	B	371	TYR	3.1
1	C	824	VAL	3.1
1	C	374	GLU	3.1
1	C	354	ASN	3.1
1	C	351	PRO	3.1
1	C	807	VAL	3.1
1	A	820	ASN	3.1
1	C	771	PRO	3.1
1	B	419	ILE	3.0
1	B	351	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	806	ILE	3.0
1	C	402	GLN	3.0
1	C	819	LEU	3.0
1	C	411	MET	2.9
1	C	820	ASN	2.9
1	C	778	VAL	2.9
1	B	806	ILE	2.9
1	B	818	SER	2.9
1	B	802	ASN	2.9
1	C	363	ALA	2.9
1	C	776	THR	2.9
1	B	767	THR	2.8
1	C	799	GLU	2.8
1	A	804	THR	2.8
1	C	392	ALA	2.8
1	C	570	LYS	2.8
1	B	810	ILE	2.7
1	C	445	GLN	2.7
1	C	790	PRO	2.7
1	C	400	LEU	2.7
1	A	452	GLN	2.7
1	A	575	LEU	2.7
1	C	635	ARG	2.7
1	B	358	SER	2.7
1	C	406	LEU	2.6
1	C	823	VAL	2.6
1	B	814	GLN	2.6
1	B	372	ILE	2.5
1	C	373	GLU	2.5
1	A	582	GLY	2.5
1	C	750	CYS	2.5
1	A	803	THR	2.5
1	B	626	GLY	2.5
1	A	776	THR	2.5
1	C	793	ILE	2.5
1	C	631	HIS	2.4
1	B	368	GLU	2.4
1	C	404	GLY	2.4
1	B	775	ASN	2.4
1	A	571	PRO	2.4
1	C	1009	TYR	2.4
1	C	571	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	776	THR	2.4
1	B	807	VAL	2.3
1	C	530	ARG	2.3
1	B	365	ILE	2.3
1	C	365	ILE	2.3
1	B	354	ASN	2.3
1	B	1008	GLU	2.3
1	B	445	GLN	2.3
1	B	769	LEU	2.3
1	C	396	LEU	2.3
1	A	777	ASP	2.3
1	C	364	ASN	2.2
1	C	951	THR	2.2
1	C	647	PRO	2.2
1	B	801	PRO	2.2
1	C	800	LEU	2.2
1	A	350	GLY	2.2
1	B	355	HIS	2.1
1	B	799	GLU	2.1
1	A	631	HIS	2.1
1	A	800	LEU	2.1
1	C	438	GLN	2.1
1	B	917	PRO	2.1
1	A	355	HIS	2.1
1	C	385	VAL	2.1
1	C	444	LEU	2.0
1	C	769	LEU	2.0
1	C	360	ASN	2.0
1	B	774	GLU	2.0
1	C	791	VAL	2.0
1	B	904	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

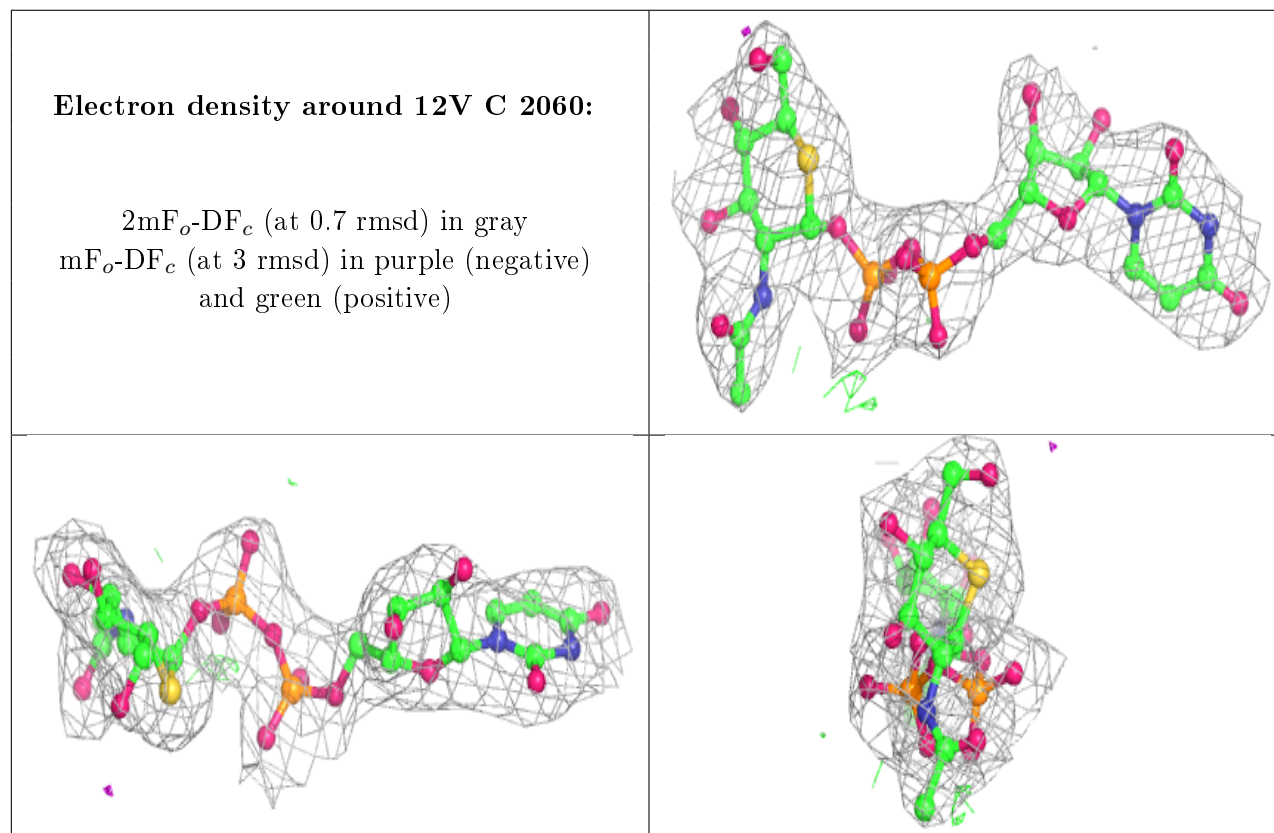
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

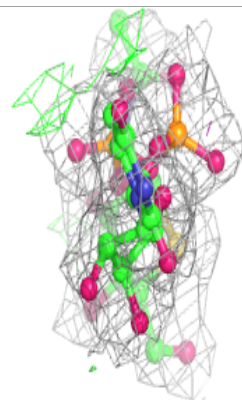
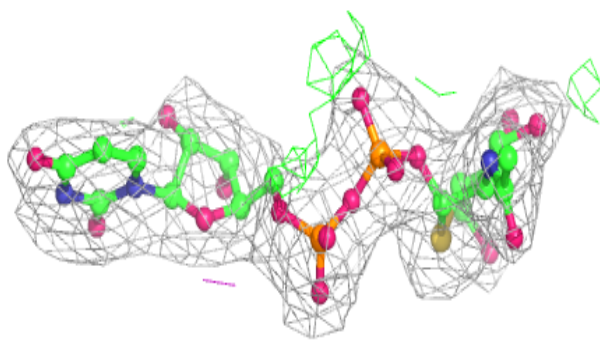
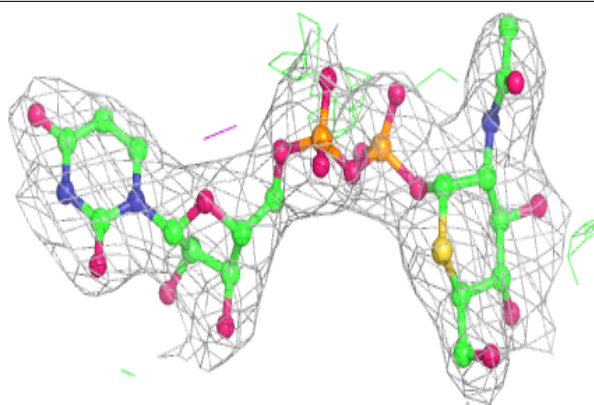
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	12V	C	2060	39/39	0.96	0.17	38,46,52,61	0
2	12V	B	2060	39/39	0.97	0.15	31,34,43,51	0
2	12V	A	2060	39/39	0.97	0.17	29,33,40,40	0

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.

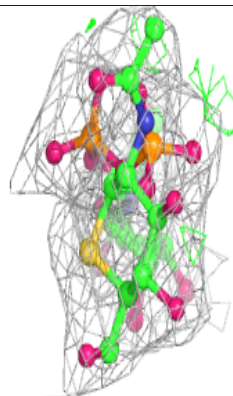
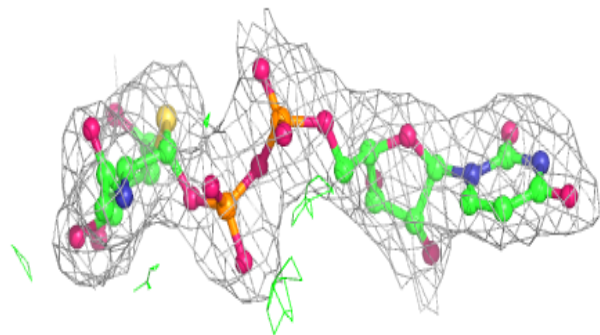
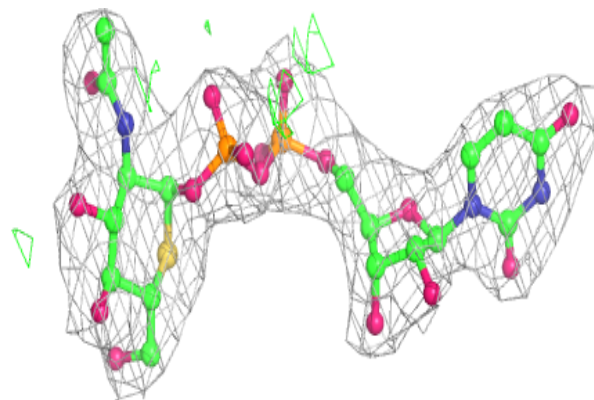


Electron density around 12V B 2060:

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

**Electron density around 12V A 2060:**

$2mF_o-DF_c$ (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.