



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2016 – 02:53 PM EDT

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
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
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) : rb-20027257

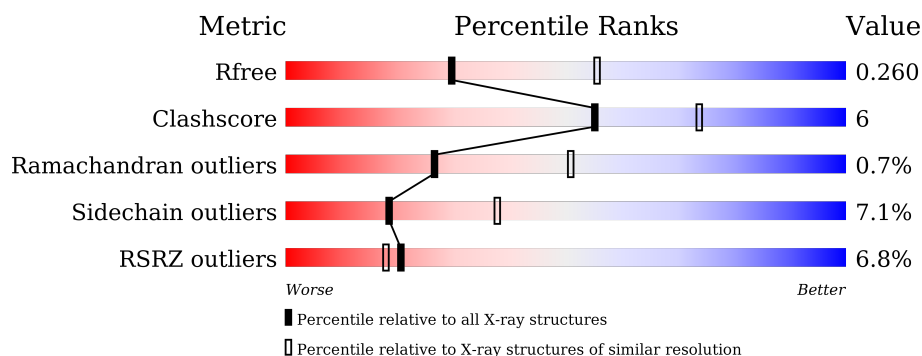
1 Overall quality at a glance

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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	710	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	710	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	C	710	<div> <div>12%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>

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.

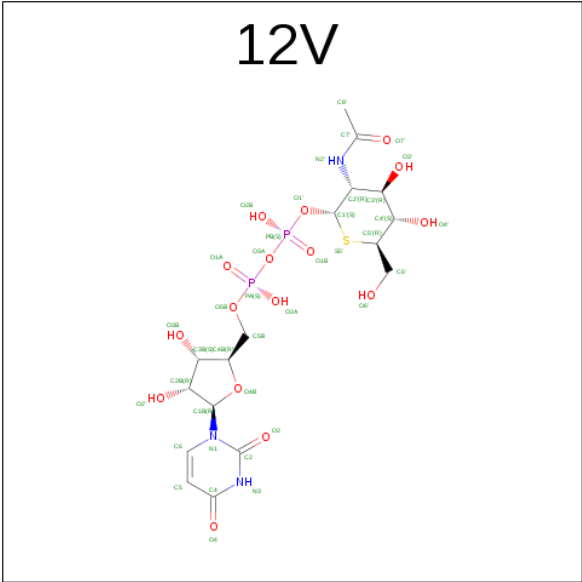
- Molecule 1 is a protein called O-GLYCOSYLTRANSFERASE.

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

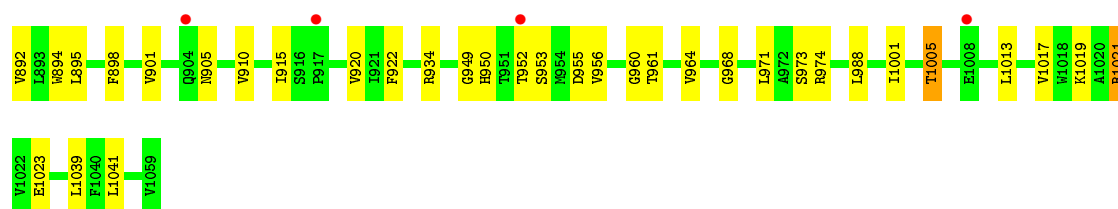
- Molecule 2 is (2S,3R,4R,5S,6R)-3-(ACETYLAMINO)-4,5-DIHYDROXY-6-(HYDROXYMETHYL)TETRAHYDRO-2H-THIOPYRAN-2-YL [(2R,3S,4R,5R)-5-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (three-letter code: 12V) (formula: C₁₇H₂₇N₃O₁₆P₂S).



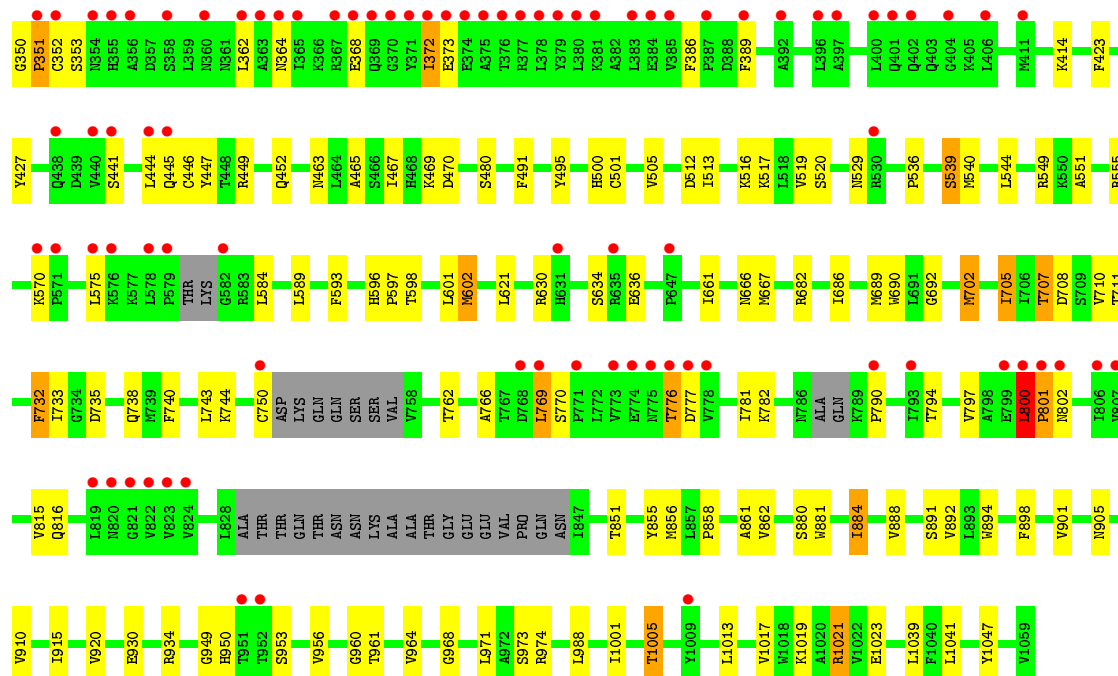
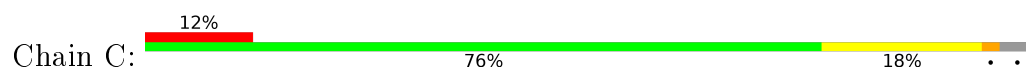
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			39	17	3	16	2	1		

- 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		



• 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 (5.33%)	DCC
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, 0.375 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: 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:988:LEU:HD21	1:C:1013:LEU:HD21	1.96	0.47
1:C:465:ALA:HB2	1:C:480:SER:CB	2.45	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:B:956:VAL:HG13	1:B:961:THR:HB	1.98	0.46
1:A:573:ASN:ND2	1:C:449:ARG:NH2	2.63	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:579:PRO:HD2	1:C:441:SER:OG	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: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:707:THR:HB	1:A:708:ASP:H	1.32	0.42
1:A:744:LYS:HA	1:A:1021:ARG:HH22	1.84	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:595:ASN:HB2	1:A:627:THR:HG21	2.03	0.41
1:A:414:LYS:NZ	1:B:659:ASP:HA	2.36	0.41
1:B:888:VAL:HA	1:B:889:PRO:HD3	1.94	0.41
1:A:578:LEU:HA	1:C:445:GLN:NE2	2.35	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%)	26	51
1	B	671/710 (94%)	648 (97%)	18 (3%)	5 (1%)	26	51
1	C	671/710 (94%)	649 (97%)	17 (2%)	5 (1%)	26	51
All	All	2013/2130 (94%)	1947 (97%)	51 (2%)	15 (1%)	26	51

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%)	17	35
1	B	583/620 (94%)	543 (93%)	40 (7%)	19	39
1	C	583/620 (94%)	542 (93%)	41 (7%)	19	38
All	All	1749/1860 (94%)	1625 (93%)	124 (7%)	18	38

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	A	2060	-	32,41,41	1.54	3 (9%)	41,62,62	1.42	3 (7%)
2	12V	B	2060	-	32,41,41	1.74	5 (15%)	41,62,62	1.50	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	12V	C	2060	-	32,41,41	1.38	4 (12%)	41,62,62	1.45	4 (9%)

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	A	2060	-	-	0/21/63/63	0/3/3/3
2	12V	B	2060	-	-	0/21/63/63	0/3/3/3
2	12V	C	2060	-	-	0/21/63/63	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2060	12V	C5'-S5'	-3.97	1.76	1.82
2	B	2060	12V	C4'-C5'	-3.55	1.50	1.53
2	C	2060	12V	C5'-S5'	-2.41	1.78	1.82
2	C	2060	12V	PB-O1'	2.37	1.67	1.60
2	B	2060	12V	O4B-C1B	2.38	1.44	1.41
2	B	2060	12V	C6'-C5'	3.07	1.54	1.52
2	A	2060	12V	C4-N3	3.87	1.40	1.33
2	C	2060	12V	C6-N1	3.93	1.40	1.35
2	C	2060	12V	C4-N3	4.04	1.40	1.33
2	A	2060	12V	C6-N1	4.07	1.41	1.35
2	B	2060	12V	C4-N3	4.45	1.41	1.33
2	B	2060	12V	C6-N1	5.01	1.42	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2060	12V	C4B-O4B-C1B	-4.81	104.55	109.64
2	B	2060	12V	C4B-O4B-C1B	-3.63	105.79	109.64
2	B	2060	12V	C5B-C4B-C3B	-2.73	104.64	115.20
2	A	2060	12V	C3'-C2'-N2'	-2.28	105.93	110.67
2	C	2060	12V	O2B-PB-O3A	2.03	113.98	105.27
2	C	2060	12V	O1'-C1'-C2'	2.26	111.08	107.39
2	B	2060	12V	C4'-C3'-C2'	2.44	114.08	110.37
2	A	2060	12V	C4'-C3'-C2'	2.92	114.81	110.37
2	B	2060	12V	O4B-C1B-N1	3.94	115.59	108.10
2	B	2060	12V	C4-N3-C2	4.69	119.15	114.21
2	C	2060	12V	C4-N3-C2	5.17	119.66	114.21

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	2060	12V	C4-N3-C2	5.64	120.15	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%) 61 59	25, 40, 70, 116	8 (1%)
1	B	681/710 (95%)	0.20	38 (5%) 28 25	21, 44, 83, 119	8 (1%)
1	C	681/710 (95%)	0.62	83 (12%) 5 4	33, 55, 102, 139	8 (1%)
All	All	2043/2130 (95%)	0.31	138 (6%) 20 18	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	7.4
1	C	440	VAL	7.1
1	C	379	TYR	6.6
1	C	441	SER	6.5
1	C	383	LEU	6.3
1	C	578	LEU	6.2
1	C	377	ARG	6.0
1	C	376	THR	5.9
1	B	820	ASN	5.8
1	C	575	LEU	5.6
1	C	801	PRO	5.3
1	C	821	GLY	5.2
1	C	352	CYS	5.1
1	C	802	ASN	5.0
1	C	777	ASP	5.0
1	C	579	PRO	4.9
1	C	371	TYR	4.6
1	C	384	GLU	4.4
1	C	375	ALA	4.3
1	C	389	PHE	4.3
1	C	370	GLY	4.3
1	C	952	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	768	ASP	4.2
1	B	777	ASP	4.0
1	C	768	ASP	4.0
1	C	367	ARG	3.9
1	A	801	PRO	3.9
1	C	576	LYS	3.8
1	B	786	ASN	3.7
1	C	582	GLY	3.7
1	C	378	LEU	3.6
1	B	785	VAL	3.6
1	C	372	ILE	3.6
1	C	358	SER	3.6
1	C	356	ALA	3.5
1	C	369	GLN	3.5
1	C	773	VAL	3.5
1	C	822	VAL	3.5
1	B	952	THR	3.5
1	C	362	LEU	3.5
1	C	401	GLN	3.5
1	B	822	VAL	3.5
1	A	821	GLY	3.4
1	C	774	GLU	3.4
1	C	775	ASN	3.3
1	A	952	THR	3.3
1	B	812	THR	3.3
1	B	821	GLY	3.3
1	C	381	LYS	3.2
1	C	387	PRO	3.2
1	C	824	VAL	3.2
1	C	368	GLU	3.2
1	C	397	ALA	3.2
1	A	917	PRO	3.1
1	B	811	ALA	3.1
1	C	351	PRO	3.1
1	B	371	TYR	3.1
1	C	374	GLU	3.1
1	C	771	PRO	3.1
1	A	820	ASN	3.1
1	C	354	ASN	3.0
1	C	807	VAL	3.0
1	B	818	SER	3.0
1	B	351	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	419	ILE	3.0
1	C	820	ASN	3.0
1	C	778	VAL	3.0
1	C	806	ILE	2.9
1	C	402	GLN	2.9
1	B	802	ASN	2.9
1	C	819	LEU	2.9
1	B	806	ILE	2.9
1	C	411	MET	2.9
1	C	776	THR	2.9
1	B	767	THR	2.8
1	C	392	ALA	2.8
1	A	575	LEU	2.8
1	C	363	ALA	2.8
1	C	799	GLU	2.8
1	A	452	GLN	2.7
1	C	790	PRO	2.7
1	C	406	LEU	2.7
1	A	804	THR	2.7
1	B	810	ILE	2.7
1	C	570	LYS	2.7
1	C	445	GLN	2.7
1	C	400	LEU	2.7
1	A	582	GLY	2.6
1	C	373	GLU	2.6
1	A	803	THR	2.6
1	C	635	ARG	2.6
1	C	823	VAL	2.6
1	C	750	CYS	2.5
1	B	814	GLN	2.5
1	B	626	GLY	2.5
1	B	358	SER	2.5
1	B	372	ILE	2.5
1	C	793	ILE	2.5
1	A	776	THR	2.5
1	A	571	PRO	2.4
1	C	1009	TYR	2.4
1	C	631	HIS	2.4
1	B	776	THR	2.4
1	C	571	PRO	2.4
1	B	775	ASN	2.4
1	C	365	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	368	GLU	2.3
1	C	404	GLY	2.3
1	C	530	ARG	2.3
1	B	807	VAL	2.3
1	B	365	ILE	2.3
1	B	354	ASN	2.3
1	C	364	ASN	2.3
1	C	396	LEU	2.3
1	B	1008	GLU	2.3
1	A	777	ASP	2.3
1	C	951	THR	2.2
1	A	350	GLY	2.2
1	B	769	LEU	2.2
1	C	800	LEU	2.2
1	B	445	GLN	2.2
1	B	801	PRO	2.2
1	A	800	LEU	2.2
1	C	385	VAL	2.1
1	B	355	HIS	2.1
1	C	438	GLN	2.1
1	A	355	HIS	2.1
1	C	647	PRO	2.1
1	A	631	HIS	2.1
1	B	799	GLU	2.1
1	C	360	ASN	2.1
1	B	917	PRO	2.1
1	C	444	LEU	2.0
1	B	774	GLU	2.0
1	C	769	LEU	2.0
1	B	904	GLN	2.0
1	B	809	MET	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 [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(\AA^2)	Q<0.9
2	12V	A	2060	39/39	0.97	0.17	-0.48	29,33,40,40	0
2	12V	C	2060	39/39	0.96	0.17	-0.60	38,46,52,61	0
2	12V	B	2060	39/39	0.97	0.15	-0.66	31,34,43,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.