Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 05:15 PM EDT

PDB ID	:	2FFV
Title	:	Human ppGalNAcT-2 complexed with manganese and UDP
Authors	:	Fritz, T.A.
Deposited on	:	2005-12-20
Resolution	:	2.75 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:

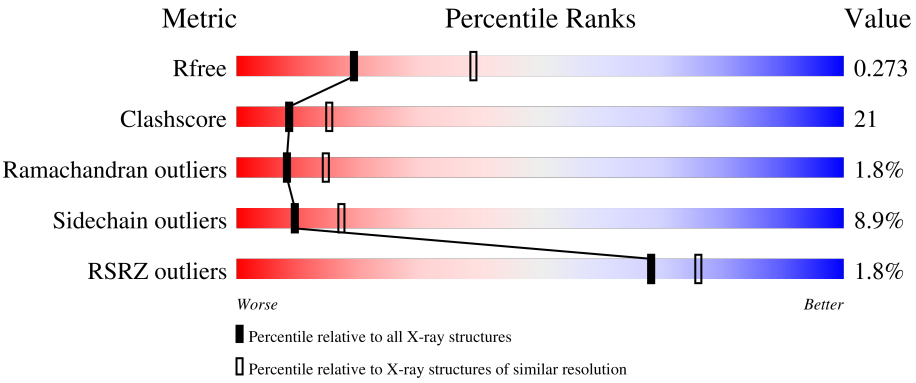
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

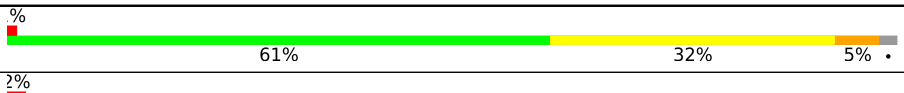
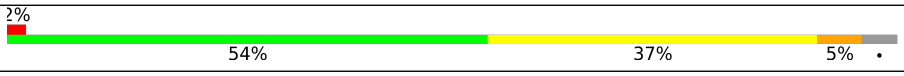
The reported resolution of this entry is 2.75 Å.

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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	501	
1	B	501	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7832 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 Polypeptide N-acetylgalactosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	31	0	0
			3921	2471	711	716	23			
1	B	481	Total	C	N	O	S	31	0	0
			3859	2432	698	706	23			

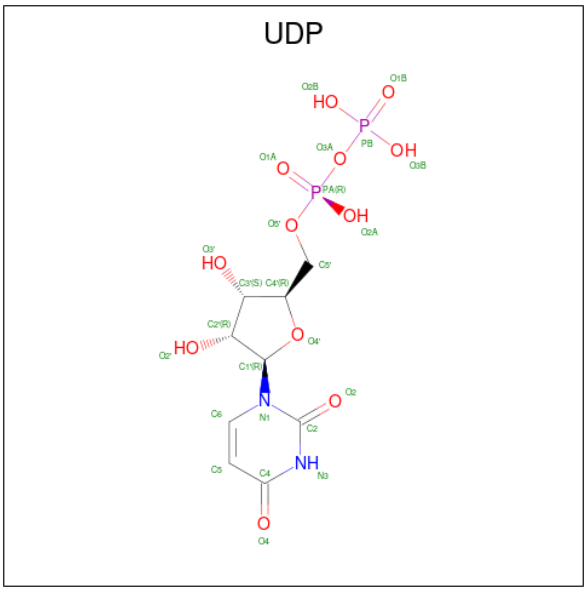
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	SER	-	cloning artifact	UNP Q10471
A	72	ASP	-	cloning artifact	UNP Q10471
A	73	ALA	-	cloning artifact	UNP Q10471
A	74	LEU	-	cloning artifact	UNP Q10471
B	71	SER	-	cloning artifact	UNP Q10471
B	72	ASP	-	cloning artifact	UNP Q10471
B	73	ALA	-	cloning artifact	UNP Q10471
B	74	LEU	-	cloning artifact	UNP Q10471

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

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



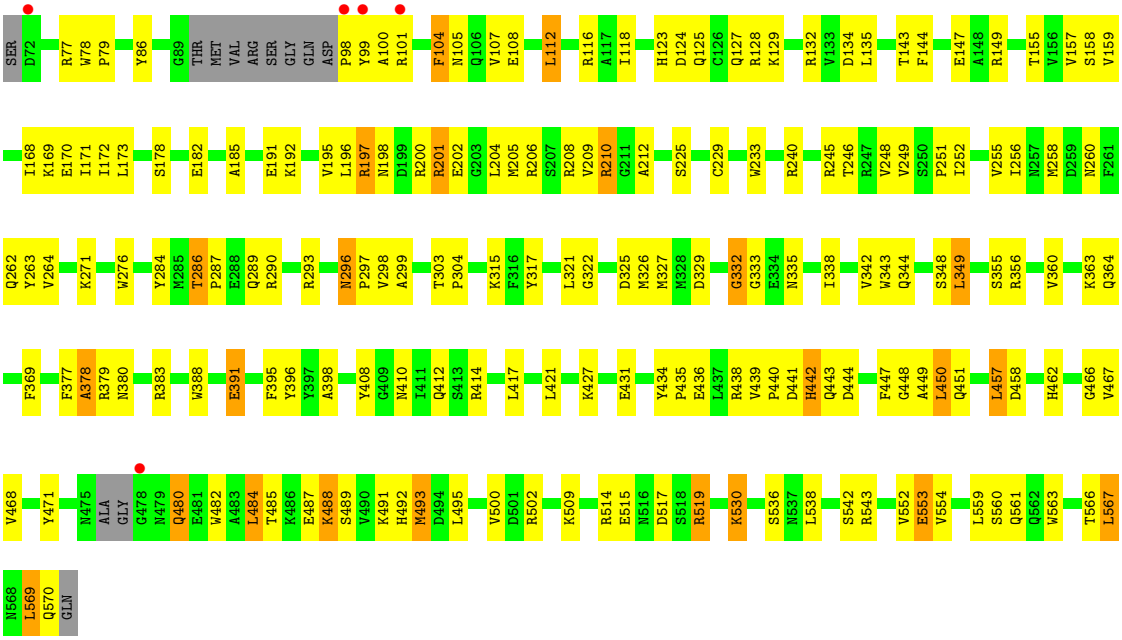
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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.

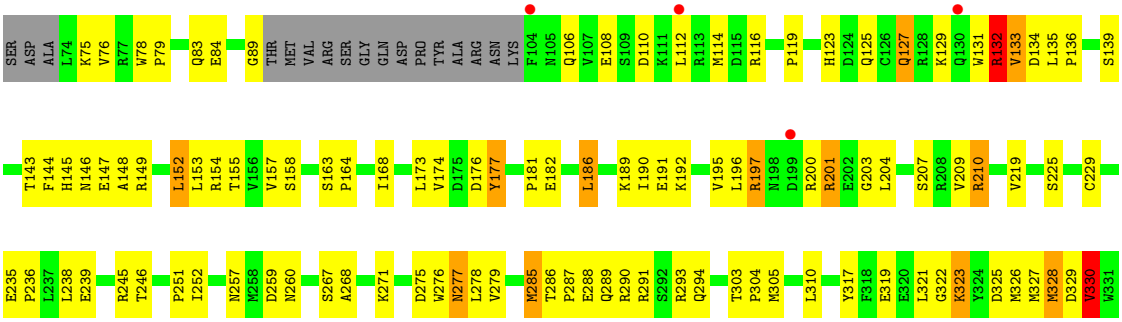
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

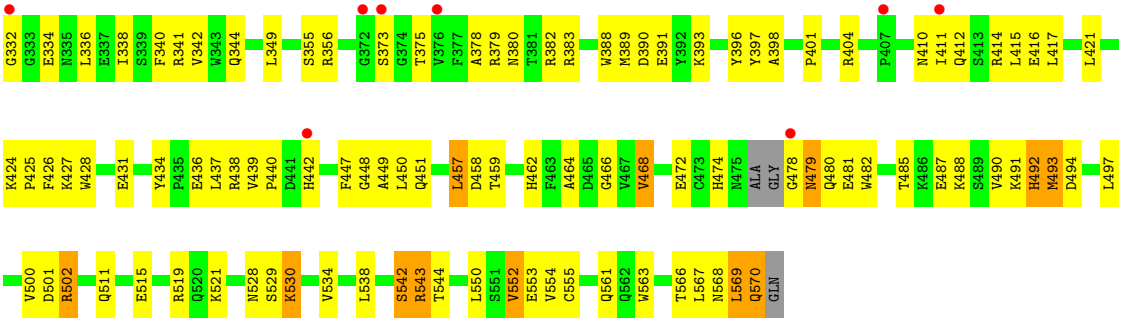
Chain A:



• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

Chain B:




G332 G333 E334 N335 L336 E337 I338 S339 F340 R341 V342 W343 Q344 L349 S355 R356 G372 S373 G374 T375 V376 F377 A378 R379 N380 T381 R382 R383 W388 M389 D390 E391 Y392 K393 Y396 Y397 A398 P401 R404 P407 M410 I411 Q412 S413 R414 L415 E416 L417 L421
K424 P425 F426 K427 W428 E431 Y434 P435 E436 L437 R438 V439 P440 D441 H442 F447 G448 A449 L450 Q451 L457 D458 T459 H462 F463 A464 D465 G466 V467 V468 E472 C473 H474 N475 ALA GLY G478 M479 Q480 E481 W482 T485 K486 E487 K488 S489 V490 K491 H492 M493 D494 L497
V500 D501 R502 Q511 E515 R519 Q520 K521 N528 S529 K530 V534 L538 S542 R543 T544 L550 S551 V552 E553 V554 C555 Q561 Q562 W563 T566 L567 N568 L569 Q570 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	153.23Å 153.23Å 110.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.75 49.09 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.10-2.75) 98.9 (49.09-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.286 0.211 , 0.273	Depositor DCC
R_{free} test set	1731 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7832	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.44	0/4011	0.67	0/5421
1	B	0.39	0/3947	0.66	1/5335 (0.0%)
All	All	0.41	0/7958	0.66	1/10756 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	492	HIS	N-CA-C	-5.61	95.86	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3921	0	3841	146	0
1	B	3859	0	3780	178	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	11	1	0
3	B	25	0	11	1	0
All	All	7832	0	7643	316	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 21.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LEU:HB3	1:A:552:VAL:HG22	1.42	0.99
1:B:450:LEU:HD23	1:B:457:LEU:HD12	1.44	0.97
1:B:257:ASN:ND2	1:B:260:ASN:H	1.64	0.96
1:B:181:PRO:HG3	1:B:197:ARG:HH21	1.32	0.92
1:B:257:ASN:HD22	1:B:260:ASN:H	0.90	0.88
1:B:181:PRO:HG3	1:B:197:ARG:NH2	1.89	0.87
1:B:153:LEU:O	1:B:157:VAL:HG12	1.76	0.86
1:A:447:PHE:O	1:A:567:LEU:HD23	1.76	0.86
1:A:128:ARG:HB2	1:A:128:ARG:NH1	1.91	0.85
1:B:257:ASN:HD22	1:B:260:ASN:N	1.73	0.84
1:B:291:ARG:O	1:B:294:GLN:HG2	1.77	0.83
1:A:329:ASP:H	1:A:380:ASN:HD21	1.24	0.82
1:B:286:THR:HG22	1:B:288:GLU:H	1.45	0.80
1:B:410:ASN:HD21	1:B:412:GLN:HB2	1.47	0.78
1:B:373:SER:HB2	1:B:375:THR:HG22	1.66	0.76
1:B:276:TRP:O	1:B:396:TYR:HA	1.86	0.75
1:A:335:ASN:HA	1:A:338:ILE:HG22	1.68	0.75
1:A:201:ARG:HH11	1:A:201:ARG:HG3	1.52	0.74
1:B:538:LEU:HB3	1:B:552:VAL:HG22	1.69	0.72
1:A:206:ARG:HG2	1:A:326:MET:HE3	1.71	0.72
1:A:123:HIS:HD2	1:A:125:GLN:HB2	1.54	0.71
1:B:332:GLY:HA3	1:B:380:ASN:HB2	1.73	0.71
1:B:329:ASP:O	1:B:330:VAL:HG12	1.92	0.69
1:B:285:MET:HE3	1:B:293:ARG:HG3	1.73	0.69
1:A:212:ALA:O	1:A:315:LYS:HE3	1.91	0.69
1:B:450:LEU:HD11	1:B:563:TRP:HB3	1.75	0.68
1:A:538:LEU:HB3	1:A:552:VAL:CG2	2.20	0.68
1:A:332:GLY:HA3	1:A:380:ASN:HB2	1.74	0.68
1:A:132:ARG:HB2	1:A:134:ASP:OD2	1.94	0.68
1:B:530:LYS:HB3	1:B:561:GLN:O	1.93	0.68
1:A:485:THR:HG21	1:A:491:LYS:HE3	1.75	0.67
1:B:286:THR:HB	1:B:289:GLN:HG3	1.78	0.66
1:B:305:MET:CE	1:B:336:LEU:HD23	2.26	0.65
1:B:252:ILE:HB	1:B:356:ARG:HD3	1.77	0.65
1:B:569:LEU:HD23	1:B:569:LEU:N	2.11	0.65
1:B:114:MET:HB2	1:B:157:VAL:HG11	1.78	0.65
1:B:144:PHE:CE2	1:B:152:LEU:HD11	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:O	1:A:290:ARG:HG3	1.97	0.64
1:B:123:HIS:HD2	1:B:125:GLN:HB2	1.63	0.64
1:A:132:ARG:O	1:A:135:LEU:HG	1.98	0.63
1:B:196:LEU:HB3	1:B:210:ARG:NH1	2.13	0.63
1:B:329:ASP:HB3	1:B:379:ARG:HD3	1.81	0.63
1:A:296:ASN:HB3	1:A:299:ALA:HB2	1.80	0.63
1:A:440:PRO:HB3	1:A:447:PHE:CG	2.34	0.63
1:B:196:LEU:HD23	1:B:210:ARG:HD2	1.81	0.63
1:B:555:CYS:HA	1:B:561:GLN:HE22	1.63	0.63
1:A:201:ARG:HG3	1:A:201:ARG:NH1	2.10	0.62
1:B:129:LYS:HB2	1:B:129:LYS:NZ	2.14	0.62
1:A:391:GLU:CD	1:A:391:GLU:H	2.01	0.62
1:B:196:LEU:HD23	1:B:210:ARG:CD	2.30	0.62
1:B:474:HIS:O	1:B:478:GLY:HA2	1.99	0.62
1:A:123:HIS:CD2	1:A:125:GLN:HB2	2.34	0.61
1:A:206:ARG:HG2	1:A:326:MET:CE	2.29	0.61
1:B:338:ILE:O	1:B:342:VAL:HG23	2.00	0.61
1:A:395:PHE:CZ	1:A:440:PRO:HG2	2.35	0.61
1:B:448:GLY:HA2	1:B:481:GLU:HG2	1.83	0.61
1:B:235:GLU:HB2	1:B:236:PRO:HD3	1.82	0.61
1:A:128:ARG:HB2	1:A:128:ARG:HH11	1.66	0.60
1:B:135:LEU:HD13	1:B:238:LEU:HB2	1.82	0.60
1:A:344:GLN:HE22	1:A:388:TRP:HB3	1.66	0.60
1:B:317:TYR:CZ	1:B:321:LEU:HD11	2.36	0.60
1:A:329:ASP:N	1:A:380:ASN:HD21	1.99	0.60
1:A:441:ASP:OD2	1:A:442:HIS:HD2	1.84	0.60
1:A:182:GLU:HA	1:A:185:ALA:HB3	1.83	0.59
1:B:174:VAL:HG11	1:B:207:SER:HB3	1.84	0.59
1:B:412:GLN:O	1:B:416:GLU:HB2	2.02	0.59
1:B:123:HIS:HD2	1:B:125:GLN:H	1.49	0.59
1:A:286:THR:HG23	1:A:287:PRO:HD2	1.85	0.58
1:B:330:VAL:HG13	1:B:330:VAL:O	2.03	0.58
1:A:204:LEU:HD21	1:A:208:ARG:HD2	1.84	0.58
1:B:123:HIS:CD2	1:B:125:GLN:H	2.21	0.58
1:A:123:HIS:CD2	1:A:125:GLN:H	2.22	0.58
1:A:128:ARG:HB2	1:A:128:ARG:CZ	2.34	0.58
1:B:440:PRO:HB3	1:B:447:PHE:CG	2.38	0.58
1:A:542:SER:HB2	1:A:560:SER:HB2	1.85	0.58
1:B:485:THR:HG21	1:B:491:LYS:HE3	1.86	0.58
1:A:98:PRO:HB3	1:A:107:VAL:HG23	1.86	0.57
1:B:286:THR:HG22	1:B:288:GLU:N	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:GLU:CD	1:B:334:GLU:H	2.07	0.57
1:A:78:TRP:CG	1:A:79:PRO:HD3	2.40	0.57
1:A:200:ARG:O	1:A:202:GLU:HG2	2.04	0.57
1:A:449:ALA:H	1:A:566:THR:HG23	1.69	0.57
1:B:480:GLN:HG2	1:B:492:HIS:CE1	2.38	0.57
1:A:155:THR:O	1:A:158:SER:HB3	2.05	0.57
1:B:257:ASN:HD21	1:B:259:ASP:HB2	1.70	0.56
1:B:132:ARG:O	1:B:133:VAL:C	2.43	0.56
1:B:257:ASN:ND2	1:B:259:ASP:H	2.04	0.56
1:B:135:LEU:HB3	1:B:136:PRO:HD2	1.88	0.56
1:B:305:MET:HE1	1:B:336:LEU:HD23	1.87	0.56
1:A:276:TRP:O	1:A:396:TYR:HA	2.05	0.56
1:B:462:HIS:HB3	1:B:466:GLY:HA3	1.88	0.56
1:A:395:PHE:CE2	1:A:440:PRO:HG2	2.41	0.55
1:B:411:ILE:HD13	1:B:415:LEU:HG	1.88	0.55
1:A:471:TYR:CE2	1:B:472:GLU:HG3	2.41	0.55
1:A:286:THR:HB	1:A:289:GLN:HG3	1.87	0.55
1:B:143:THR:CG2	1:B:204:LEU:HD12	2.37	0.55
1:B:209:VAL:HG13	1:B:323:LYS:HE3	1.88	0.55
1:A:447:PHE:O	1:A:567:LEU:CD2	2.53	0.55
1:B:191:GLU:O	1:B:192:LYS:HG2	2.05	0.55
1:B:321:LEU:O	1:B:341:ARG:HD2	2.07	0.55
1:B:277:ASN:C	1:B:277:ASN:HD22	2.09	0.55
1:B:285:MET:CE	1:B:293:ARG:HG3	2.36	0.54
1:B:246:THR:HA	1:B:317:TYR:CE1	2.42	0.54
1:A:124:ASP:O	1:A:127:GLN:HB3	2.08	0.54
1:A:168:ILE:HG22	1:A:168:ILE:O	2.06	0.54
1:B:528:ASN:HB3	1:B:568:ASN:ND2	2.23	0.54
1:B:135:LEU:HD22	1:B:239:GLU:HA	1.88	0.53
1:B:383:ARG:CZ	1:B:411:ILE:HG22	2.39	0.53
1:B:450:LEU:CD2	1:B:457:LEU:HD12	2.29	0.53
1:A:559:LEU:HD12	1:A:559:LEU:N	2.24	0.53
1:B:427:LYS:HE3	1:B:431:GLU:OE1	2.08	0.53
1:B:132:ARG:HD2	1:B:135:LEU:HD23	1.91	0.53
1:A:260:ASN:OD1	1:A:262:GLN:HB2	2.08	0.53
1:B:131:TRP:CH2	1:B:236:PRO:HG3	2.44	0.53
1:A:191:GLU:O	1:A:192:LYS:HB2	2.09	0.52
1:B:201:ARG:HG3	1:B:201:ARG:HH11	1.73	0.52
1:A:500:VAL:HG21	1:A:509:LYS:HG3	1.91	0.52
1:B:330:VAL:HG22	3:B:9601:UDP:O2'	2.09	0.52
1:A:264:VAL:HG13	1:B:511:GLN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:TRP:O	1:B:426:PHE:HB2	2.09	0.52
1:A:335:ASN:HA	1:A:338:ILE:CG2	2.37	0.52
1:A:530:LYS:HB3	1:A:561:GLN:O	2.10	0.52
1:B:78:TRP:CG	1:B:79:PRO:HD3	2.44	0.52
1:A:248:VAL:HB	1:A:349:LEU:HD12	1.92	0.52
1:B:340:PHE:HB3	1:B:344:GLN:NE2	2.25	0.51
1:A:159:VAL:HG12	1:A:168:ILE:HD13	1.91	0.51
1:B:155:THR:O	1:B:158:SER:HB3	2.11	0.51
1:B:277:ASN:HD22	1:B:278:LEU:N	2.08	0.51
1:A:108:GLU:O	1:A:112:LEU:HD22	2.10	0.51
1:A:143:THR:HG23	3:A:5601:UDP:H5	1.74	0.51
1:B:459:THR:HG23	1:B:480:GLN:OE1	2.11	0.51
1:B:490:VAL:HG11	1:B:497:LEU:HD12	1.93	0.51
1:A:514:ARG:HH22	1:B:119:PRO:HG3	1.75	0.51
1:B:322:GLY:HA3	1:B:417:LEU:HD21	1.92	0.51
1:A:255:VAL:HG21	1:B:464:ALA:HB1	1.92	0.51
1:B:424:LYS:HB3	1:B:425:PRO:HD2	1.93	0.51
1:A:205:MET:O	1:A:209:VAL:HG23	2.11	0.51
1:A:471:TYR:HE2	1:B:472:GLU:HG3	1.74	0.51
1:B:389:MET:HA	1:B:426:PHE:CG	2.46	0.51
1:A:159:VAL:HG12	1:A:168:ILE:CD1	2.41	0.51
1:A:488:LYS:HA	1:A:488:LYS:HE3	1.93	0.51
1:A:492:HIS:O	1:A:493:MET:HB2	2.11	0.51
1:A:438:ARG:HH12	1:B:290:ARG:NH2	2.09	0.51
1:B:209:VAL:CG1	1:B:323:LYS:HE3	2.40	0.51
1:B:487:GLU:O	1:B:488:LYS:HB2	2.11	0.50
1:B:186:LEU:HD22	1:B:189:LYS:NZ	2.25	0.50
1:B:410:ASN:ND2	1:B:412:GLN:HB2	2.22	0.50
1:A:286:THR:HG22	1:A:289:GLN:H	1.76	0.50
1:B:201:ARG:HG3	1:B:201:ARG:NH1	2.26	0.50
1:B:285:MET:HE1	1:B:293:ARG:NH1	2.26	0.50
1:A:379:ARG:HG3	1:A:408:TYR:HA	1.94	0.50
1:B:132:ARG:HD2	1:B:135:LEU:CD2	2.42	0.49
1:A:229:CYS:HB3	1:A:233:TRP:CD1	2.47	0.49
1:B:251:PRO:HB3	1:B:355:SER:OG	2.11	0.49
1:B:425:PRO:O	1:B:428:TRP:HB3	2.12	0.49
1:A:271:LYS:HD3	1:A:289:GLN:OE1	2.13	0.49
1:B:147:GLU:HG3	1:B:148:ALA:N	2.28	0.49
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.78	0.49
1:A:204:LEU:CD2	1:A:208:ARG:HD2	2.43	0.49
1:A:343:TRP:CH2	1:A:348:SER:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ARG:NH1	1:A:536:SER:HB3	2.27	0.49
1:B:319:GLU:HA	1:B:323:LYS:HG3	1.94	0.49
1:A:132:ARG:HH11	1:A:134:ASP:CG	2.16	0.49
1:B:145:HIS:O	1:B:146:ASN:HB2	2.13	0.49
1:B:277:ASN:C	1:B:277:ASN:ND2	2.66	0.49
1:A:338:ILE:O	1:A:342:VAL:HG23	2.13	0.49
1:A:447:PHE:HB3	1:A:567:LEU:HD21	1.93	0.49
1:B:89:GLY:HA3	1:B:149:ARG:NH1	2.27	0.49
1:A:178:SER:O	1:A:197:ARG:NH2	2.46	0.48
1:B:143:THR:HG21	1:B:204:LEU:HD12	1.95	0.48
1:A:128:ARG:HH11	1:A:128:ARG:CB	2.26	0.48
1:A:209:VAL:HG21	1:A:326:MET:SD	2.53	0.48
1:A:325:ASP:CG	1:A:414:ARG:HD2	2.33	0.48
1:B:182:GLU:HG3	1:B:186:LEU:HG	1.94	0.48
1:B:123:HIS:CD2	1:B:125:GLN:HB2	2.45	0.48
1:A:104:PHE:HB2	1:A:258:MET:HB2	1.95	0.48
1:B:154:ARG:O	1:B:158:SER:HB2	2.14	0.48
1:A:251:PRO:HB3	1:A:355:SER:OG	2.14	0.48
1:B:410:ASN:HD21	1:B:412:GLN:CB	2.22	0.48
1:A:327:MET:HB2	1:A:383:ARG:NH2	2.29	0.48
1:B:305:MET:HE3	1:B:336:LEU:HD23	1.96	0.48
1:B:329:ASP:O	1:B:330:VAL:CG1	2.62	0.48
1:B:534:VAL:O	1:B:534:VAL:HG13	2.13	0.47
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.49	0.47
1:B:325:ASP:O	1:B:328:MET:HG3	2.14	0.47
1:B:502:ARG:HG2	1:B:502:ARG:HH11	1.78	0.47
1:A:129:LYS:HB2	1:A:129:LYS:NZ	2.29	0.47
1:B:191:GLU:C	1:B:192:LYS:HG2	2.34	0.47
1:B:457:LEU:HD22	1:B:482:TRP:CZ2	2.49	0.47
1:B:286:THR:HG23	1:B:287:PRO:HD2	1.95	0.47
1:B:414:ARG:O	1:B:417:LEU:HB3	2.14	0.47
1:A:517:ASP:CG	1:A:519:ARG:HE	2.18	0.47
1:B:568:ASN:C	1:B:570:GLN:H	2.18	0.47
1:A:495:LEU:HD21	1:B:267:SER:HB2	1.96	0.46
1:B:275:ASP:HB2	1:B:277:ASN:ND2	2.30	0.46
1:B:391:GLU:H	1:B:391:GLU:CD	2.19	0.46
1:B:468:VAL:O	1:B:550:LEU:HG	2.16	0.46
1:A:284:TYR:HD2	1:B:493:MET:HE1	1.80	0.46
1:A:246:THR:HA	1:A:317:TYR:CE1	2.51	0.46
1:B:329:ASP:HB3	1:B:379:ARG:CD	2.45	0.46
1:A:364:GLN:HG2	1:A:369:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:PRO:HG2	1:B:219:VAL:HG21	1.98	0.46
1:A:170:GLU:HG3	1:A:172:ILE:HG13	1.98	0.46
1:B:411:ILE:HD12	1:B:411:ILE:C	2.36	0.46
1:A:462:HIS:HD2	1:A:467:VAL:O	1.98	0.46
1:B:397:TYR:CD1	1:B:404:ARG:HG2	2.50	0.46
1:A:514:ARG:HB2	1:A:517:ASP:HB2	1.98	0.46
1:A:378:ALA:O	1:A:379:ARG:C	2.54	0.46
1:A:86:TYR:CE2	1:A:149:ARG:HB3	2.51	0.45
1:B:252:ILE:HD12	1:B:268:ALA:HA	1.98	0.45
1:A:327:MET:HA	1:A:327:MET:CE	2.47	0.45
1:B:158:SER:OG	1:B:229:CYS:N	2.49	0.45
1:B:457:LEU:HD11	1:B:497:LEU:HD11	1.97	0.45
1:A:144:PHE:HB3	1:A:225:SER:HB3	1.99	0.45
1:A:240:ARG:HB2	1:A:249:VAL:HG11	1.99	0.45
1:A:252:ILE:HB	1:A:356:ARG:HD3	1.99	0.45
1:B:257:ASN:ND2	1:B:260:ASN:N	2.46	0.45
1:B:398:ALA:CB	1:B:569:LEU:HD22	2.47	0.45
1:A:123:HIS:HD2	1:A:125:GLN:CB	2.25	0.45
1:A:286:THR:HG23	1:A:287:PRO:CD	2.46	0.45
1:B:401:PRO:O	1:B:404:ARG:HG3	2.17	0.45
1:B:542:SER:O	1:B:544:THR:N	2.50	0.45
1:B:457:LEU:HD23	1:B:458:ASP:N	2.32	0.45
1:B:382:ARG:HD2	1:B:397:TYR:OH	2.16	0.45
1:A:448:GLY:HA3	1:A:566:THR:OG1	2.17	0.44
1:B:329:ASP:O	1:B:330:VAL:CB	2.66	0.44
1:A:293:ARG:HA	1:A:296:ASN:O	2.16	0.44
1:A:377:PHE:CD2	1:A:377:PHE:N	2.85	0.44
1:A:377:PHE:H	1:A:377:PHE:HD2	1.65	0.44
1:A:458:ASP:HA	1:A:480:GLN:OE1	2.18	0.44
1:B:182:GLU:OE1	1:B:186:LEU:HD23	2.16	0.44
1:B:382:ARG:HD3	1:B:397:TYR:HE1	1.83	0.44
1:A:77:ARG:HB3	1:A:79:PRO:HD2	1.98	0.44
1:B:543:ARG:HG3	1:B:543:ARG:HH11	1.82	0.44
1:A:256:ILE:CG2	1:A:360:VAL:HG22	2.45	0.44
1:A:519:ARG:HG2	1:A:519:ARG:HH11	1.82	0.44
1:B:144:PHE:CD1	1:B:144:PHE:C	2.91	0.44
1:B:447:PHE:CG	1:B:448:GLY:N	2.85	0.44
1:A:98:PRO:HG2	1:A:99:TYR:CD2	2.52	0.44
1:B:321:LEU:HD23	1:B:421:LEU:HD13	2.00	0.44
1:A:147:GLU:HG2	1:A:225:SER:HB2	1.99	0.44
1:A:296:ASN:HD22	1:A:297:PRO:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LEU:HD23	1:A:567:LEU:H	1.82	0.44
1:B:177:TYR:HD2	1:B:201:ARG:N	2.16	0.43
1:B:145:HIS:CD2	1:B:201:ARG:NH2	2.86	0.43
1:A:344:GLN:NE2	1:A:388:TRP:HB3	2.31	0.43
1:A:333:GLY:C	1:A:335:ASN:N	2.70	0.43
1:A:538:LEU:HA	1:A:553:GLU:O	2.18	0.43
1:A:487:GLU:O	1:A:488:LYS:HB2	2.18	0.43
1:B:127:GLN:H	1:B:127:GLN:HG2	1.46	0.43
1:B:569:LEU:N	1:B:569:LEU:CD2	2.81	0.43
1:A:321:LEU:HA	1:A:321:LEU:HD23	1.80	0.43
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.83	0.43
1:B:176:ASP:OD1	1:B:203:GLY:N	2.49	0.43
1:A:240:ARG:CB	1:A:249:VAL:HG11	2.49	0.43
1:A:484:LEU:HA	1:A:489:SER:O	2.18	0.43
1:A:104:PHE:CB	1:A:258:MET:HB2	2.49	0.43
1:A:78:TRP:CD1	1:A:79:PRO:HD3	2.54	0.42
1:A:128:ARG:NH1	1:A:128:ARG:CB	2.74	0.42
1:A:134:ASP:OD2	1:A:134:ASP:N	2.49	0.42
1:A:159:VAL:CG1	1:A:168:ILE:HD13	2.48	0.42
1:A:450:LEU:HD13	1:A:563:TRP:CE3	2.54	0.42
1:B:277:ASN:ND2	1:B:279:VAL:H	2.17	0.42
1:A:303:THR:HA	1:A:304:PRO:HD3	1.88	0.42
1:B:277:ASN:HD22	1:B:277:ASN:N	2.16	0.42
1:A:488:LYS:HA	1:A:488:LYS:CE	2.50	0.42
1:A:296:ASN:ND2	1:A:298:VAL:H	2.17	0.42
1:A:329:ASP:H	1:A:380:ASN:ND2	2.02	0.42
1:A:398:ALA:CB	1:A:569:LEU:HD23	2.50	0.42
1:A:449:ALA:H	1:A:566:THR:CG2	2.33	0.42
1:B:449:ALA:N	1:B:566:THR:HG23	2.35	0.42
1:A:427:LYS:HE3	1:A:431:GLU:OE1	2.20	0.42
1:B:390:ASP:O	1:B:393:LYS:HG2	2.20	0.42
1:B:479:ASN:N	1:B:479:ASN:OD1	2.52	0.42
1:A:444:ASP:O	1:A:569:LEU:HD12	2.20	0.42
1:A:552:VAL:O	1:A:552:VAL:HG13	2.20	0.42
1:B:83:GLN:NE2	1:B:114:MET:HG2	2.35	0.42
1:B:538:LEU:HA	1:B:553:GLU:O	2.19	0.42
1:B:78:TRP:CD1	1:B:79:PRO:HD3	2.54	0.42
1:A:271:LYS:HE3	1:A:271:LYS:HB2	1.82	0.41
1:B:135:LEU:H	1:B:135:LEU:HG	1.63	0.41
1:B:493:MET:HB2	1:B:494:ASP:H	1.57	0.41
1:A:569:LEU:O	1:A:570:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:VAL:CG1	1:B:497:LEU:HD12	2.51	0.41
1:B:521:LYS:HB3	1:B:534:VAL:HG11	2.02	0.41
1:A:198:ASN:ND2	1:A:210:ARG:NH1	2.68	0.41
1:B:76:VAL:HG12	1:B:189:LYS:O	2.20	0.41
1:B:108:GLU:O	1:B:112:LEU:HD23	2.20	0.41
1:B:144:PHE:HB3	1:B:225:SER:HB3	2.03	0.41
1:A:118:ILE:HD12	1:A:263:TYR:CE2	2.56	0.41
1:A:171:ILE:HG22	1:A:173:LEU:CD1	2.50	0.41
1:B:303:THR:HA	1:B:304:PRO:HD3	1.91	0.41
1:B:75:LYS:HE3	1:B:190:ILE:O	2.20	0.41
1:B:84:GLU:OE2	1:B:84:GLU:HA	2.20	0.41
1:B:129:LYS:HB2	1:B:129:LYS:HZ2	1.81	0.41
1:B:168:ILE:O	1:B:192:LYS:HE2	2.21	0.41
1:A:410:ASN:OD1	1:A:412:GLN:HB2	2.21	0.41
1:A:256:ILE:HB	1:A:360:VAL:HG22	2.02	0.41
1:A:442:HIS:CD2	1:A:443:GLN:HG3	2.56	0.41
1:A:462:HIS:HB3	1:A:466:GLY:HA3	2.02	0.41
1:B:293:ARG:HG3	1:B:293:ARG:NH1	2.34	0.41
1:B:434:TYR:CE2	1:B:437:LEU:HB2	2.56	0.41
1:B:438:ARG:HH21	1:B:438:ARG:HG2	1.86	0.41
1:A:204:LEU:C	1:A:204:LEU:HD23	2.41	0.41
1:A:434:TYR:N	1:A:435:PRO:CD	2.84	0.41
1:B:163:SER:HA	1:B:164:PRO:HD3	1.90	0.40
1:B:277:ASN:ND2	1:B:277:ASN:H	2.20	0.40
1:B:378:ALA:O	1:B:379:ARG:C	2.58	0.40
1:B:383:ARG:NH2	1:B:411:ILE:HG22	2.36	0.40
1:B:529:SER:C	1:B:530:LYS:HG2	2.41	0.40
1:A:322:GLY:HA3	1:A:417:LEU:HD21	2.02	0.40
1:A:123:HIS:HD2	1:A:125:GLN:H	1.69	0.40
1:B:132:ARG:HB3	1:B:135:LEU:HD21	2.03	0.40
1:B:186:LEU:HD22	1:B:189:LYS:HZ3	1.85	0.40
1:B:252:ILE:CD1	1:B:268:ALA:HA	2.52	0.40
1:B:440:PRO:HB3	1:B:447:PHE:CD1	2.57	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	483/501 (96%)	446 (92%)	27 (6%)	10 (2%)	7 12
1	B	475/501 (95%)	427 (90%)	41 (9%)	7 (2%)	10 18
All	All	958/1002 (96%)	873 (91%)	68 (7%)	17 (2%)	8 15

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLU
1	B	132	ARG
1	B	133	VAL
1	B	330	VAL
1	B	515	GLU
1	A	101	ARG
1	A	543	ARG
1	B	543	ARG
1	A	100	ALA
1	A	104	PHE
1	A	105	ASN
1	A	332	GLY
1	A	363	LYS
1	B	323	LYS
1	B	326	MET
1	A	378	ALA
1	A	493	MET

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	422/433 (98%)	391 (93%)	31 (7%)	14 25
1	B	417/433 (96%)	373 (89%)	44 (11%)	6 11
All	All	839/866 (97%)	764 (91%)	75 (9%)	9 17

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	116	ARG
1	A	157	VAL
1	A	169	LYS
1	A	195	VAL
1	A	196	LEU
1	A	197	ARG
1	A	201	ARG
1	A	210	ARG
1	A	245	ARG
1	A	286	THR
1	A	296	ASN
1	A	349	LEU
1	A	391	GLU
1	A	421	LEU
1	A	436	GLU
1	A	439	VAL
1	A	442	HIS
1	A	450	LEU
1	A	451	GLN
1	A	457	LEU
1	A	468	VAL
1	A	480	GLN
1	A	484	LEU
1	A	488	LYS
1	A	519	ARG
1	A	530	LYS
1	A	553	GLU
1	A	554	VAL
1	A	567	LEU
1	A	569	LEU
1	B	106	GLN
1	B	110	ASP
1	B	116	ARG

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Mol	Chain	Res	Type
1	B	127	GLN
1	B	132	ARG
1	B	134	ASP
1	B	139	SER
1	B	152	LEU
1	B	173	LEU
1	B	177	TYR
1	B	186	LEU
1	B	195	VAL
1	B	197	ARG
1	B	200	ARG
1	B	201	ARG
1	B	210	ARG
1	B	245	ARG
1	B	271	LYS
1	B	277	ASN
1	B	285	MET
1	B	310	LEU
1	B	327	MET
1	B	328	MET
1	B	330	VAL
1	B	349	LEU
1	B	436	GLU
1	B	439	VAL
1	B	442	HIS
1	B	451	GLN
1	B	457	LEU
1	B	468	VAL
1	B	479	ASN
1	B	493	MET
1	B	500	VAL
1	B	501	ASP
1	B	502	ARG
1	B	519	ARG
1	B	530	LYS
1	B	542	SER
1	B	552	VAL
1	B	554	VAL
1	B	567	LEU
1	B	569	LEU
1	B	570	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	198	ASN
1	A	296	ASN
1	A	344	GLN
1	A	364	GLN
1	A	380	ASN
1	A	442	HIS
1	A	443	GLN
1	A	451	GLN
1	A	452	GLN
1	A	462	HIS
1	A	474	HIS
1	A	570	GLN
1	B	123	HIS
1	B	179	ASN
1	B	198	ASN
1	B	232	HIS
1	B	257	ASN
1	B	277	ASN
1	B	294	GLN
1	B	296	ASN
1	B	344	GLN
1	B	364	GLN
1	B	394	ASN
1	B	410	ASN
1	B	432	ASN
1	B	442	HIS
1	B	443	GLN
1	B	451	GLN
1	B	462	HIS
1	B	474	HIS
1	B	524	GLN
1	B	533	HIS
1	B	561	GLN
1	B	568	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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
3	UDP	B	9601	2	24,26,26	2.79	7 (29%)	37,40,40	2.18	12 (32%)
3	UDP	A	5601	2	24,26,26	2.67	8 (33%)	37,40,40	2.13	11 (29%)

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
3	UDP	B	9601	2	-	7/16/32/32	0/2/2/2
3	UDP	A	5601	2	-	2/16/32/32	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9601	UDP	C6-C5	8.47	1.54	1.35
3	A	5601	UDP	C6-C5	8.10	1.53	1.35
3	B	9601	UDP	C6-N1	5.76	1.51	1.38
3	A	5601	UDP	C6-N1	5.51	1.51	1.38
3	B	9601	UDP	C3'-C4'	-4.74	1.40	1.53
3	A	5601	UDP	C3'-C4'	-4.35	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9601	UDP	C2-N1	4.20	1.45	1.38
3	B	9601	UDP	C5-C4	4.02	1.52	1.43
3	A	5601	UDP	C2-N1	3.91	1.44	1.38
3	A	5601	UDP	C5-C4	3.36	1.51	1.43
3	A	5601	UDP	C4-N3	2.64	1.43	1.38
3	A	5601	UDP	PA-O1A	-2.26	1.42	1.50
3	B	9601	UDP	PA-O1A	-2.22	1.43	1.50
3	B	9601	UDP	C4-N3	2.20	1.42	1.38
3	A	5601	UDP	O4-C4	-2.03	1.20	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5601	UDP	C5-C4-N3	5.17	122.57	114.84
3	B	9601	UDP	O2'-C2'-C1'	5.14	127.19	110.02
3	B	9601	UDP	C5-C4-N3	5.09	122.45	114.84
3	A	5601	UDP	O2'-C2'-C1'	5.04	126.87	110.02
3	A	5601	UDP	C6-C5-C4	-4.38	113.53	119.52
3	B	9601	UDP	C6-C5-C4	-4.32	113.61	119.52
3	B	9601	UDP	N3-C2-N1	4.11	120.34	114.89
3	A	5601	UDP	O4-C4-C5	-3.85	118.39	125.16
3	A	5601	UDP	N3-C2-N1	3.82	119.96	114.89
3	B	9601	UDP	O3B-PB-O3A	3.57	116.62	104.64
3	B	9601	UDP	O4-C4-C5	-3.39	119.19	125.16
3	A	5601	UDP	O3B-PB-O3A	3.30	115.69	104.64
3	B	9601	UDP	O4'-C1'-C2'	-3.25	99.56	106.64
3	A	5601	UDP	O4'-C1'-C2'	-3.09	99.91	106.64
3	A	5601	UDP	C2'-C1'-N1	-2.95	104.85	113.22
3	B	9601	UDP	C3'-C2'-C1'	-2.86	95.99	101.43
3	B	9601	UDP	O2'-C2'-C3'	-2.46	103.85	111.82
3	A	5601	UDP	C4-N3-C2	-2.40	123.42	126.58
3	B	9601	UDP	C2'-C1'-N1	-2.30	106.69	113.22
3	B	9601	UDP	C4-N3-C2	-2.28	123.58	126.58
3	A	5601	UDP	C3'-C2'-C1'	-2.23	97.19	101.43
3	A	5601	UDP	O3'-C3'-C2'	2.17	118.83	111.82
3	B	9601	UDP	O3'-C3'-C2'	2.13	118.72	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	9601	UDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	B	9601	UDP	O4'-C4'-C5'-O5'
3	B	9601	UDP	C5'-O5'-PA-O2A
3	B	9601	UDP	C5'-O5'-PA-O3A
3	B	9601	UDP	PB-O3A-PA-O1A
3	B	9601	UDP	C5'-O5'-PA-O1A
3	A	5601	UDP	PB-O3A-PA-O1A
3	A	5601	UDP	PB-O3A-PA-O2A
3	B	9601	UDP	PB-O3A-PA-O2A

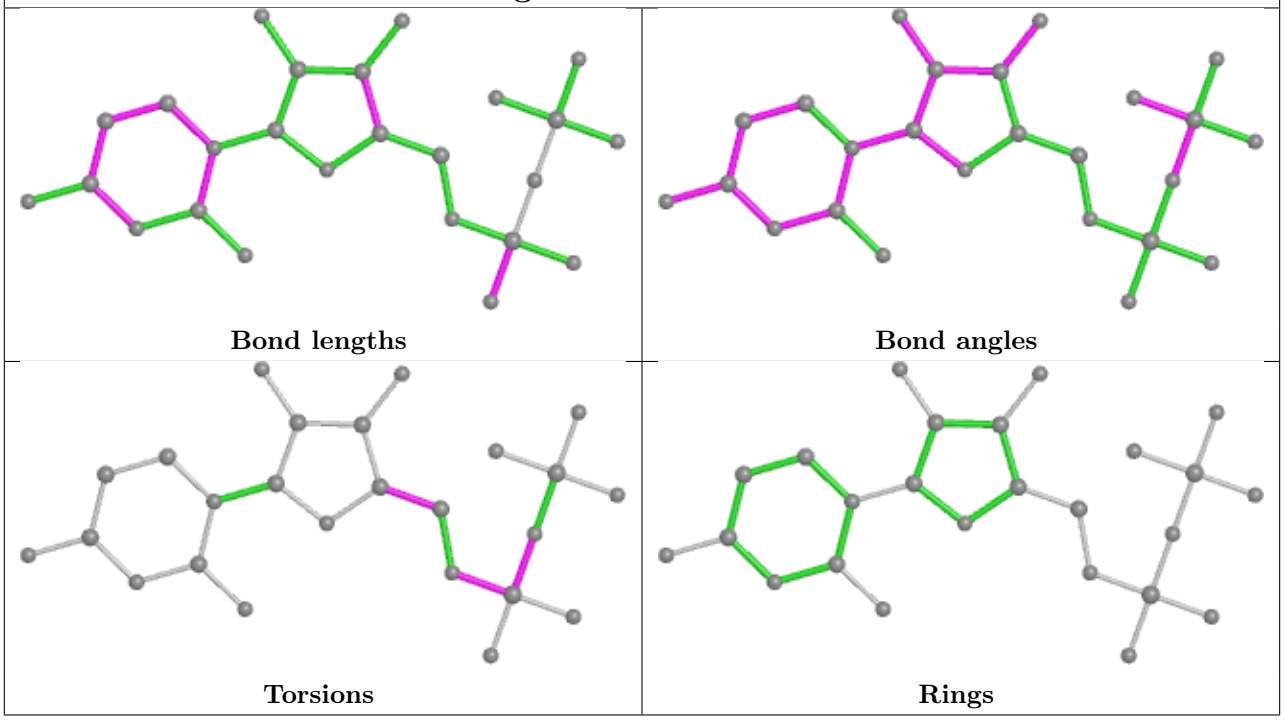
There are no ring outliers.

2 monomers are involved in 2 short contacts:

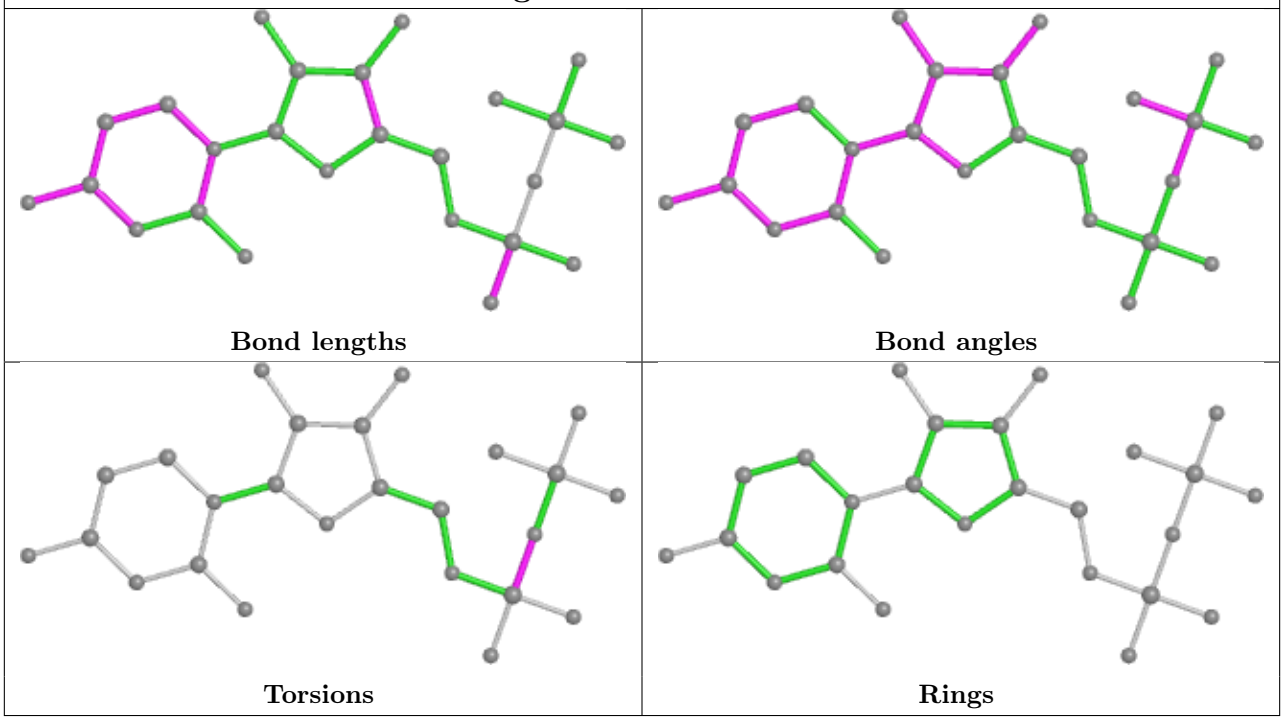
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	9601	UDP	1	0
3	A	5601	UDP	1	0

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 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 UDP B 9601



Ligand UDP A 5601



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, 95^{th} 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	489/501 (97%)	-0.22	5 (1%)	82	87	17, 36, 72, 113	8 (1%)
1	B	481/501 (96%)	0.02	12 (2%)	57	66	18, 42, 84, 127	8 (1%)
All	All	970/1002 (96%)	-0.10	17 (1%)	68	76	17, 39, 79, 127	16 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	PRO	4.0
1	B	373	SER	3.8
1	B	411	ILE	3.2
1	B	372	GLY	3.2
1	A	72	ASP	2.9
1	A	99	TYR	2.8
1	A	478	GLY	2.8
1	B	478	GLY	2.8
1	B	130	GLN	2.8
1	B	332	GLY	2.6
1	B	442	HIS	2.2
1	B	407	PRO	2.1
1	B	112	LEU	2.1
1	B	199	ASP	2.1
1	B	104	PHE	2.1
1	A	101	ARG	2.0
1	B	376	VAL	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

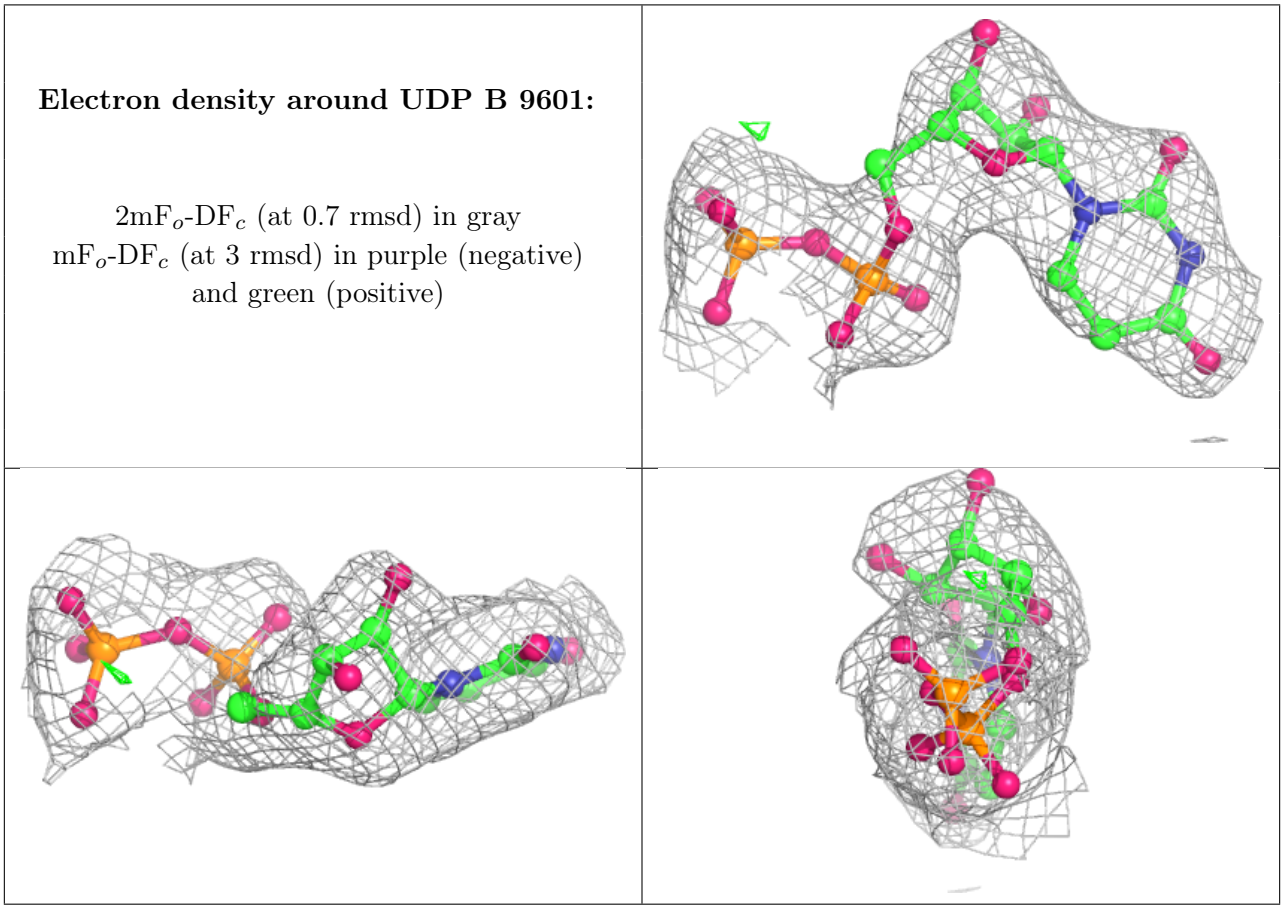
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	UDP	B	9601	25/25	0.96	0.14	58,67,68,68	0
3	UDP	A	5601	25/25	0.97	0.14	43,47,49,51	0
2	MN	A	5600	1/1	0.99	0.10	23,23,23,23	0
2	MN	B	9600	1/1	0.99	0.07	39,39,39,39	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.

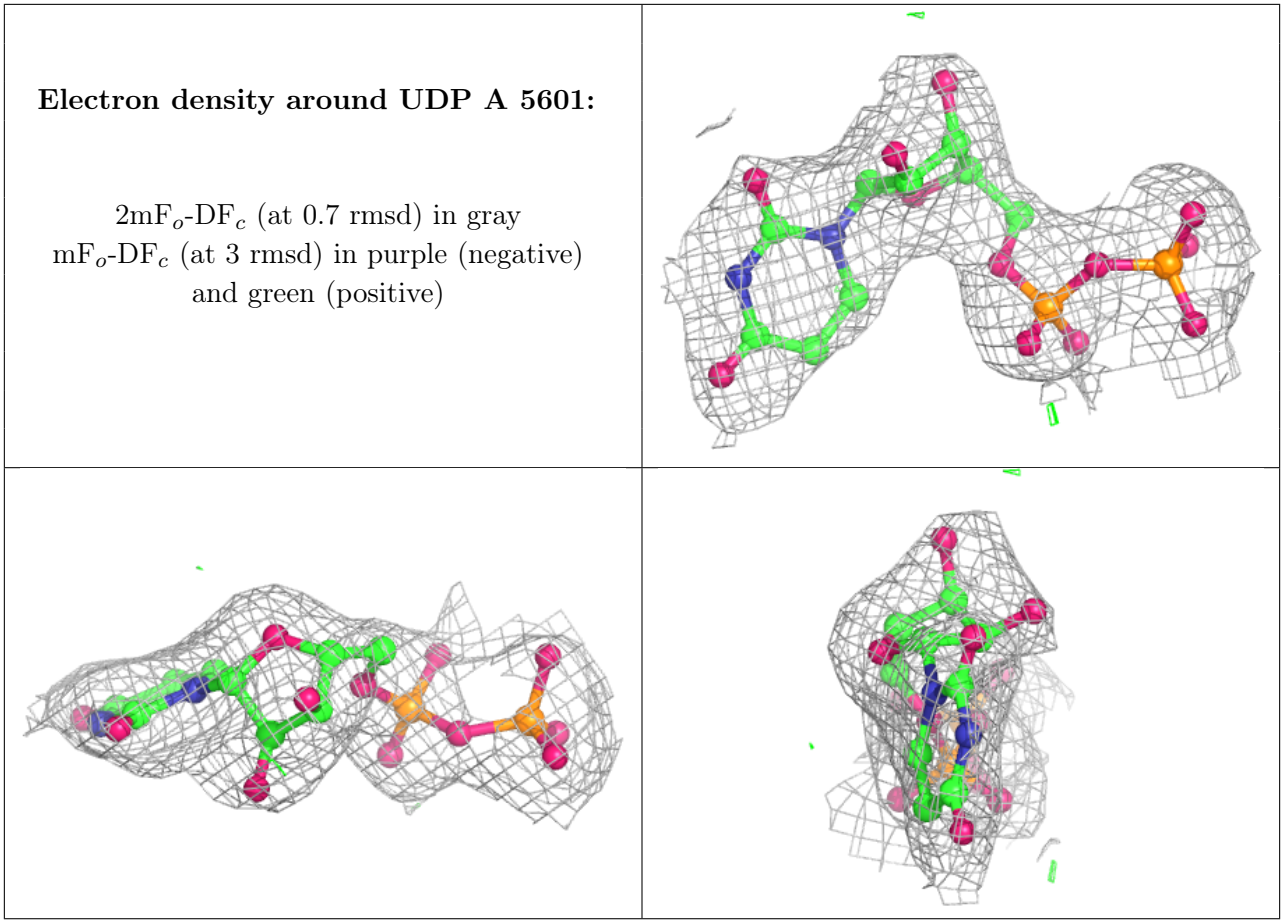
Electron density around UDP B 9601:

$2mF_o$-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 5601:

$2mF_o$-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.