



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:46 am GMT

PDB ID : 3PE4
Title : Structure of human O-GlcNAc transferase and its complex with a peptide substrate
Authors : Lazarus, M.B.; Nam, Y.; Jiang, J.; Sliz, P.; Walker, S.
Deposited on : 2010-10-25
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

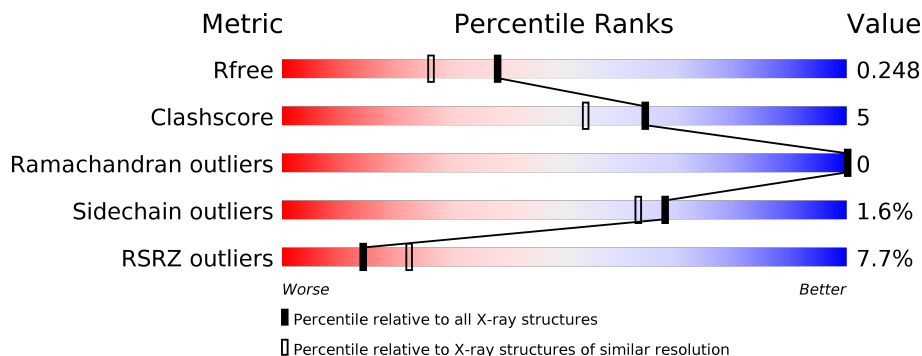
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	723	<div> <div>7%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	C	723	<div> <div>8%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
2	B	14	<div> <div>79%</div> <div>21%</div> </div>
2	D	14	<div> <div>79%</div> <div>21%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12036 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	9	0
			5549	3527	966	1019	37			
1	C	674	Total	C	N	O	S	0	8	0
			5378	3427	933	981	37			

There are 8 discrepancies between the modelled and reference sequences:

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

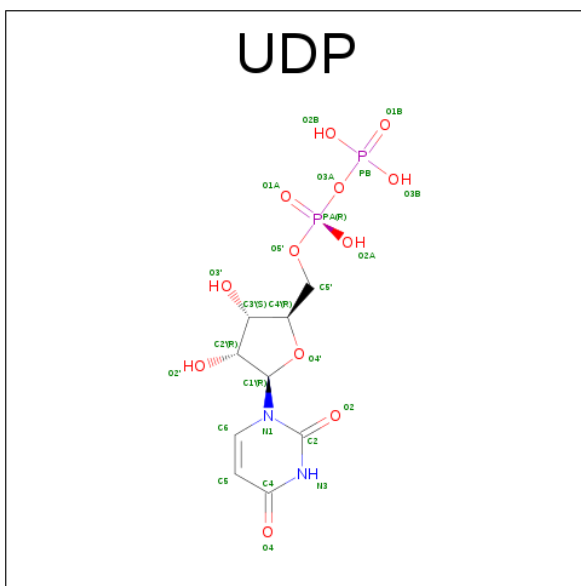
- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			
2	D	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			

There are 2 discrepancies between the modelled and reference sequences:

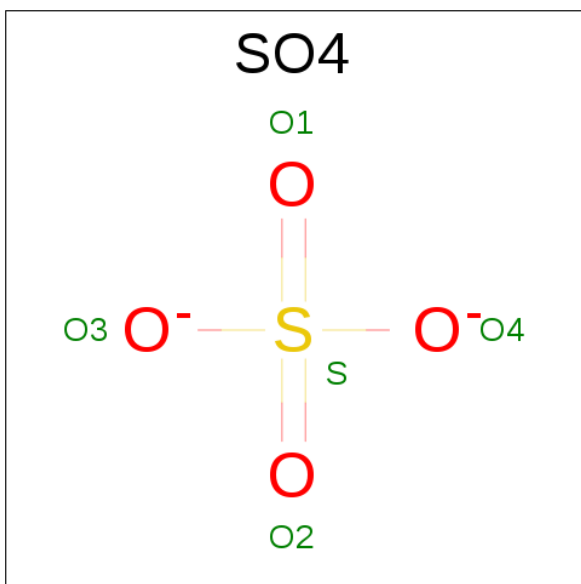
Chain	Residue	Modelled	Actual	Comment	Reference
B	13	TYR	-	EXPRESSION TAG	UNP P68400
D	13	TYR	-	EXPRESSION TAG	UNP P68400

- 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	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		


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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	412	Total	O	0	0
			412	412		
5	B	12	Total	O	0	0
			12	12		
5	C	415	Total	O	0	0
			415	415		
5	D	15	Total	O	0	0
			15	15		

Chain B:  79% 21%



- Molecule 2: Casein kinase II subunit alpha

Chain D:  79% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.60Å 136.70Å 153.50Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-1.95) 98.3 (29.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.224 , 0.252 0.219 , 0.248	Depositor DCC
R_{free} test set	7091 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12036	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 28.64 % 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 1.7790e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: UDP, SO4

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	0.37	0/5687	0.51	0/7714
1	C	0.37	0/5515	0.52	0/7482
2	B	0.34	0/97	0.53	0/131
2	D	0.36	0/97	0.52	0/131
All	All	0.37	0/11396	0.51	0/15458

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5549	0	5542	55	0
1	C	5378	0	5382	48	0
2	B	95	0	88	2	0
2	D	95	0	88	2	0
3	A	25	0	11	0	0
3	C	25	0	11	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	412	0	0	6	0
5	B	12	0	0	0	0
5	C	415	0	0	9	0
5	D	15	0	0	0	0
All	All	12036	0	11122	107	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 5.

All (107) 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:763:ASN:HA	5:C:1249:HOH:O	1.50	1.11
1:C:854[B]:ILE:HD11	1:C:967:GLU:HA	1.49	0.92
1:A:854[B]:ILE:HD11	1:A:967:GLU:HA	1.51	0.91
1:A:723:ARG:O	1:A:724[B]:ILE:HD13	1.84	0.78
1:C:723:ARG:O	1:C:724[B]:ILE:HD13	1.85	0.77
1:A:545:ARG:HD3	1:A:573:PRO:O	1.90	0.72
1:C:854[B]:ILE:HD11	1:C:967:GLU:CA	2.20	0.71
1:C:545:ARG:HD3	1:C:573:PRO:O	1.92	0.70
1:A:1028:LYS:HE2	5:A:1143:HOH:O	1.92	0.67
1:A:854[B]:ILE:HD11	1:A:967:GLU:CA	2.22	0.65
2:D:13:TYR:N	2:D:18:THR:HG1	1.95	0.65
2:B:13:TYR:N	2:B:18:THR:HG1	1.98	0.60
1:C:746:MET:N	5:C:1249:HOH:O	2.37	0.57
1:A:456:TYR:CZ	1:A:478:LYS:HD3	2.40	0.57
1:C:456:TYR:CZ	1:C:478:LYS:HD3	2.40	0.56
1:A:726:LEU:HD23	1:A:819[A]:VAL:HG22	1.87	0.56
1:C:707:LYS:HE2	1:C:762:LEU:HD22	1.88	0.56
1:A:954:GLY:O	1:A:986:LYS:HE2	2.06	0.55
1:C:726:LEU:CD2	1:C:819[A]:VAL:HG22	2.37	0.55
1:A:726:LEU:CD2	1:A:819[A]:VAL:HG22	2.37	0.55
1:C:726:LEU:HD23	1:C:819[A]:VAL:HG22	1.88	0.54
1:A:707:LYS:HE2	1:A:762:LEU:HD22	1.89	0.54
1:A:843[B]:ILE:HD11	1:A:848:LEU:HB2	1.90	0.54
1:C:770:ASN:HB2	5:C:1170:HOH:O	2.08	0.54
1:C:954:GLY:O	1:C:986:LYS:HE2	2.07	0.54
1:A:381[B]:SER:HB2	1:A:384:PHE:HB2	1.91	0.53
1:C:827[A]:LEU:HD23	1:C:891:ILE:HD12	1.91	0.53
1:C:443:ARG:NE	5:C:1260:HOH:O	2.42	0.52
1:C:843[B]:ILE:HD11	1:C:848:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:LEU:HD23	1:A:819[B]:VAL:HG12	1.92	0.52
1:A:726:LEU:CD2	1:A:819[B]:VAL:HG12	2.40	0.52
1:A:443:ARG:NH1	5:A:1257:HOH:O	2.39	0.52
1:A:854[B]:ILE:HD12	1:A:971:VAL:HG23	1.91	0.51
1:C:381[B]:SER:HB2	1:C:384:PHE:HB2	1.92	0.51
1:A:780:ILE:HD11	1:A:819[B]:VAL:CG2	2.41	0.51
1:C:780:ILE:HD11	1:C:819[B]:VAL:CG2	2.40	0.51
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.46	0.51
1:C:854[B]:ILE:HD12	1:C:971:VAL:HG23	1.92	0.51
1:C:408:TYR:CZ	1:C:424:ASN:HB3	2.47	0.50
1:C:780:ILE:HD11	1:C:819[B]:VAL:HG21	1.93	0.50
1:C:726:LEU:CD2	1:C:819[B]:VAL:HG12	2.41	0.50
1:C:762:LEU:HD23	5:C:1201:HOH:O	2.11	0.49
1:A:780:ILE:HD11	1:A:819[B]:VAL:HG21	1.94	0.49
1:A:827[A]:LEU:HD23	1:A:891:ILE:HD12	1.95	0.49
1:C:357:LEU:HD23	1:C:373:HIS:CE1	2.47	0.49
1:A:558:HIS:CG	1:A:559:PRO:HD2	2.47	0.48
1:C:825:TYR:HB2	1:C:827[B]:LEU:HD13	1.95	0.48
1:C:726:LEU:HD23	1:C:819[B]:VAL:HG12	1.94	0.48
1:A:825:TYR:HB2	1:A:827[B]:LEU:HD13	1.96	0.48
1:A:867:ARG:HB3	1:A:870:ALA:HA	1.95	0.48
1:C:558:HIS:CG	1:C:559:PRO:HD2	2.49	0.48
1:A:850:MET:SD	1:A:963:ARG:HG2	2.54	0.47
1:C:930:GLY:HA2	1:C:987:VAL:HG12	1.95	0.47
1:C:712:ASP:O	1:C:769:MET:HB2	2.14	0.47
1:A:762:LEU:HD23	5:A:1135:HOH:O	2.15	0.47
1:A:712:ASP:O	1:A:769:MET:HB2	2.15	0.47
1:A:930:GLY:HA2	1:A:987:VAL:HG12	1.97	0.47
1:A:844:ASP:HB2	1:A:845:PRO:HD2	1.97	0.46
1:C:713:PHE:HD1	1:C:713:PHE:H	1.64	0.46
1:C:850:MET:SD	1:C:963:ARG:HG2	2.55	0.46
1:C:629:MET:O	1:C:654:GLY:HA3	2.16	0.46
1:A:713:PHE:HD1	1:A:713:PHE:H	1.64	0.46
1:C:745:LYS:HA	5:C:1249:HOH:O	2.15	0.46
1:C:456:TYR:CE1	1:C:478:LYS:HD3	2.51	0.46
1:A:822:ARG:HG2	1:A:827[B]:LEU:HD23	1.96	0.46
1:A:629:MET:O	1:A:654:GLY:HA3	2.16	0.45
1:C:822:ARG:HG2	1:C:827[B]:LEU:HD23	1.99	0.45
1:A:449:LYS:HD2	5:A:1261:HOH:O	2.16	0.45
1:C:724[B]:ILE:CD1	1:C:821:THR:HB	2.46	0.44
1:C:867:ARG:HB3	1:C:870:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:ASN:HB3	1:C:842:LYS:HD2	1.99	0.44
1:C:844:ASP:HB2	1:C:845:PRO:HD2	2.00	0.44
1:A:838:ASN:HB3	1:A:842:LYS:HD2	2.00	0.44
1:C:719:ILE:N	5:C:1243:HOH:O	2.51	0.44
1:A:977:LEU:HD22	5:A:1242:HOH:O	2.17	0.44
1:A:724[B]:ILE:CD1	1:A:821:THR:HB	2.48	0.44
1:C:785:ILE:HD12	1:C:799:ALA:HB1	2.00	0.43
1:A:854[B]:ILE:CD1	1:A:971:VAL:HG23	2.48	0.43
1:A:769:MET:HG3	1:A:769:MET:O	2.19	0.43
1:A:456:TYR:CE1	1:A:478:LYS:HD3	2.52	0.43
1:A:357:LEU:HD23	1:A:373:HIS:CE1	2.54	0.43
1:C:603:ILE:N	1:C:603:ILE:HD12	2.34	0.43
1:A:603:ILE:N	1:A:603:ILE:HD12	2.34	0.43
1:C:437:GLU:HG3	5:C:307:HOH:O	2.18	0.43
1:C:337:VAL:O	1:C:341:ARG:HG3	2.19	0.42
1:A:437:GLU:HG3	5:A:1061:HOH:O	2.19	0.42
1:A:785:ILE:HD12	1:A:799:ALA:HB1	2.01	0.42
1:A:840:LEU:O	1:A:843[B]:ILE:HG23	2.20	0.42
1:A:405:LEU:HD12	1:A:428:ILE:HG21	2.01	0.42
1:C:405:LEU:HD12	1:C:428:ILE:HG21	2.01	0.42
1:C:822:ARG:HB3	1:C:827[B]:LEU:HB2	2.02	0.42
1:C:793:SER:HB3	5:C:1244:HOH:O	2.20	0.41
1:A:675:PRO:O	1:A:678:VAL:HG22	2.20	0.41
1:A:822:ARG:HB3	1:A:827[B]:LEU:HB2	2.02	0.41
1:A:723:ARG:C	1:A:724[B]:ILE:HD13	2.38	0.41
2:D:25:MET:HA	2:D:25:MET:CE	2.51	0.41
1:A:694:PHE:CZ	1:A:920:HIS:HB3	2.55	0.41
1:A:714:LYS:HE2	1:A:714:LYS:HB2	1.86	0.41
1:A:724[B]:ILE:HD12	1:A:821:THR:HB	2.03	0.41
1:A:720:TYR:HB3	1:A:723:ARG:HD3	2.03	0.41
1:A:844:ASP:HB2	1:A:845:PRO:CD	2.51	0.41
2:B:25:MET:HA	2:B:25:MET:CE	2.51	0.40
1:A:337:VAL:O	1:A:341:ARG:HG3	2.20	0.40
1:A:704:HIS:O	1:A:727:ASN:HB3	2.22	0.40
1:C:779:MET:HA	1:C:784:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	698/723 (96%)	682 (98%)	16 (2%)	0	100	100
1	C	676/723 (94%)	661 (98%)	15 (2%)	0	100	100
2	B	12/14 (86%)	12 (100%)	0	0	100	100
2	D	12/14 (86%)	12 (100%)	0	0	100	100
All	All	1398/1474 (95%)	1367 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	606/618 (98%)	597 (98%)	9 (2%)	70	65
1	C	587/618 (95%)	577 (98%)	10 (2%)	66	60
2	B	11/11 (100%)	11 (100%)	0	100	100
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	1215/1258 (97%)	1196 (98%)	19 (2%)	68	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	PHE
1	A	386	ASP

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Mol	Chain	Res	Type
1	A	452	PHE
1	A	694	PHE
1	A	713	PHE
1	A	793	SER
1	A	868	PHE
1	A	926	VAL
1	A	1028	LYS
1	C	350	PHE
1	C	384	PHE
1	C	386	ASP
1	C	452	PHE
1	C	694	PHE
1	C	713	PHE
1	C	793	SER
1	C	868	PHE
1	C	926	VAL
1	C	1028	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	364	GLN
1	A	406	GLN
1	A	681	GLN
1	C	363	GLN
1	C	406	GLN
1	C	498	HIS
1	C	681	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	UDP	A	1212	-	21,26,26	1.18	1 (4%)	22,40,40	1.73	1 (4%)
4	SO4	A	5	-	4,4,4	0.17	0	6,6,6	0.08	0
4	SO4	B	1	-	4,4,4	0.13	0	6,6,6	0.13	0
3	UDP	C	1212	-	21,26,26	1.13	1 (4%)	22,40,40	1.62	1 (4%)
4	SO4	D	3	-	4,4,4	0.19	0	6,6,6	0.15	0

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	A	1212	-	-	0/12/32/32	0/2/2/2
4	SO4	A	5	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1	-	-	0/0/0/0	0/0/0/0
3	UDP	C	1212	-	-	0/12/32/32	0/2/2/2
4	SO4	D	3	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1212	UDP	C4-N3	3.11	1.38	1.33
3	C	1212	UDP	C4-N3	3.41	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1212	UDP	C4-N3-C2	7.00	120.14	114.13
3	A	1212	UDP	C4-N3-C2	7.50	120.57	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	695/723 (96%)	0.41	50 (7%) 16 25	7, 18, 46, 73	0
1	C	674/723 (93%)	0.44	57 (8%) 11 18	7, 17, 44, 73	0
2	B	14/14 (100%)	-0.04	0 100 100	10, 17, 36, 46	0
2	D	14/14 (100%)	-0.18	0 100 100	9, 17, 36, 46	0
All	All	1397/1474 (94%)	0.41	107 (7%) 14 22	7, 18, 46, 73	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	PHE	6.8
1	C	339	LEU	6.6
1	C	348	PRO	6.5
1	C	337	VAL	6.3
1	C	338	ARG	6.1
1	C	344	LEU	5.6
1	A	713	PHE	5.4
1	C	346	VAL	5.4
1	A	315	THR	5.1
1	A	335	GLU	4.8
1	C	526	ASN	4.6
1	C	342	LYS	4.6
1	C	527	VAL	4.6
1	A	526	ASN	4.4
1	A	332	ASN	4.4
1	C	340	TYR	4.3
1	C	713	PHE	4.1
1	C	714	LYS	3.9
1	A	769	MET	3.9
1	A	746	MET	3.8
1	C	860	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	357	LEU	3.7
1	A	714	LYS	3.6
1	C	350	PHE	3.6
1	C	819[A]	VAL	3.5
1	C	529	HIS	3.5
1	C	345	GLU	3.4
1	A	384	PHE	3.4
1	C	746	MET	3.4
1	A	488	GLU	3.3
1	A	316	HIS	3.3
1	C	1027	ILE	3.2
1	C	383	THR	3.2
1	A	772	ILE	3.1
1	C	1019	ALA	3.0
1	A	331	GLY	3.0
1	C	884	GLY	3.0
1	C	360	VAL	3.0
1	A	490	ASN	3.0
1	A	529	HIS	2.9
1	A	739	PRO	2.9
1	C	353	ALA	2.9
1	A	330	GLN	2.9
1	A	742	LYS	2.9
1	A	860	ASN	2.8
1	C	843[A]	ILE	2.8
1	A	745	LYS	2.8
1	C	745	LYS	2.8
1	C	541	LEU	2.8
1	C	676	ALA	2.6
1	C	384	PHE	2.6
1	A	318	ASP	2.6
1	C	543	ASP	2.6
1	A	491	ARG	2.5
1	A	712	ASP	2.5
1	C	677	GLU	2.5
1	A	827[A]	LEU	2.5
1	C	740	ASP	2.5
1	A	383	THR	2.5
1	A	333	ILE	2.4
1	C	1006	LEU	2.4
1	A	484	ALA	2.4
1	A	843[A]	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	739	PRO	2.4
1	A	887	GLN	2.4
1	A	540	LYS	2.3
1	A	1019	ALA	2.3
1	C	769	MET	2.3
1	A	532	PRO	2.3
1	A	668	ILE	2.3
1	C	886	PRO	2.3
1	C	550	TYR	2.3
1	C	336	ALA	2.3
1	C	532	PRO	2.3
1	A	543	ASP	2.3
1	A	819[A]	VAL	2.2
1	C	356	ASN	2.2
1	A	884	GLY	2.2
1	A	319[A]	SER	2.2
1	C	341	ARG	2.2
1	A	323	LEU	2.2
1	A	609	PRO	2.2
1	A	740	ASP	2.2
1	C	668	ILE	2.2
1	C	523	ASP	2.2
1	C	1022	LYS	2.2
1	C	1020	GLY	2.1
1	A	677	GLU	2.1
1	C	361	LEU	2.1
1	C	887	GLN	2.1
1	C	399	GLN	2.1
1	C	607	GLN	2.1
1	C	525	ILE	2.1
1	A	344	LEU	2.1
1	A	507	HIS	2.1
1	A	528	LEU	2.1
1	C	763	ASN	2.1
1	A	854[A]	ILE	2.1
1	C	662	LEU	2.1
1	A	763	ASN	2.0
1	C	427	SER	2.0
1	A	348	PRO	2.0
1	A	326	ILE	2.0
1	C	798	LEU	2.0
1	A	678	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1018	ALA	2.0
1	A	1006	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	B	1	5/5	0.98	0.18	1.51	20,25,37,38	0
4	SO4	D	3	5/5	0.98	0.13	0.27	25,26,41,41	0
3	UDP	C	1212	25/25	0.98	0.08	-1.16	5,9,11,15	0
3	UDP	A	1212	25/25	0.98	0.08	-1.21	3,9,12,13	0
4	SO4	A	5	5/5	0.95	0.31	-	48,55,60,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.