



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:23 PM GMT

PDB ID : 4F4C
Title : The Crystal Structure of the Multi-Drug Transporter
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Deposited on : 2012-05-10
Resolution : 3.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

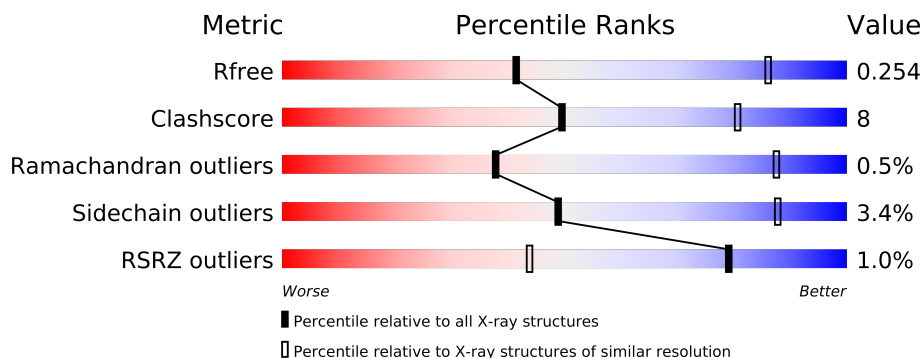
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1321	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	OSA	A	1405	-	X
3	OSA	A	1406	-	X

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9541 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

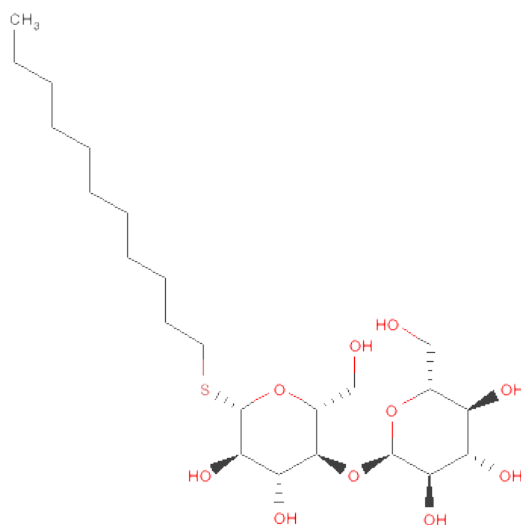
- Molecule 1 is a protein called Multidrug resistance protein pgp-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1250	Total	C	N	O	S	0	0	0
			9423	6011	1593	1772	47			

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 3 is UNDECYL 4-O-ALPHA-D-GLUCOPYRANOSYL-1-THIO-BETA-D-GLUCOPYRANOSIDE (three-letter code: OSA) (formula: C₂₃H₄₄O₁₀S).



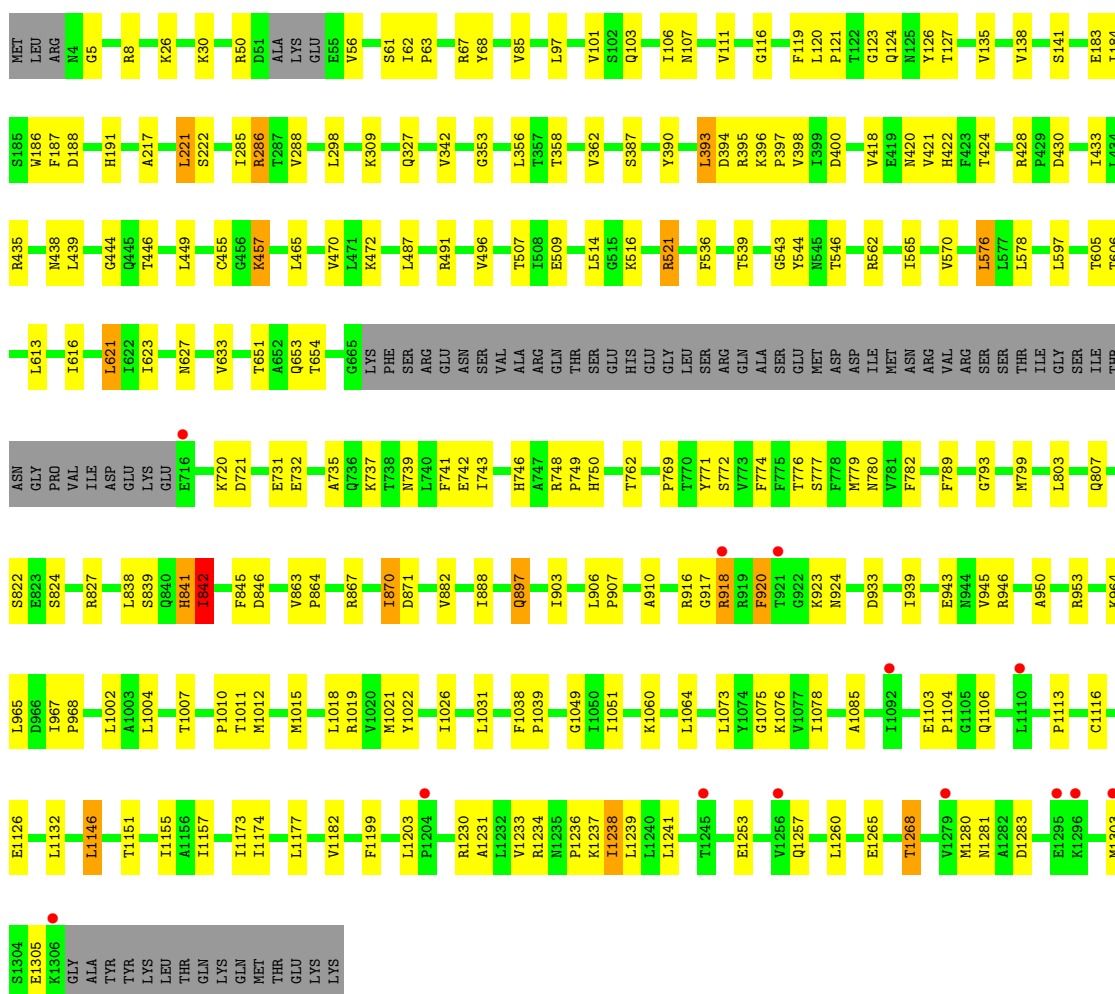
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			34	23	10	1		
3	A	1	Total	C	O	S	0	0
			34	23	10	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Multidrug resistance protein pgp-1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.90Å 155.36Å 162.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.43 – 3.40 46.43 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.43-3.40) 98.7 (46.43-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.250 , 0.283 0.250 , 0.254	Depositor DCC
R_{free} test set	1719 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	140.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.9	EDS
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33973 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9541	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0SA, BMA, NAG, NDG, MAN

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	0.43	0/9581	0.59	0/12993

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9423	0	9395	140	0
2	A	50	0	43	2	0
3	A	68	0	88	7	0
All	All	9541	0	9526	144	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (144) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:444:GLY:H	1:A:605:THR:HG22	1.10	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:521:ARG:HH11	1:A:521:ARG:HG3	1.37	0.89
1:A:920:PHE:O	1:A:920:PHE:HD1	1.54	0.89
1:A:56:VAL:HG11	1:A:387:SER:OG	1.79	0.81
1:A:621:LEU:HD11	1:A:633:VAL:HG13	1.64	0.80
1:A:1126:GLU:HG3	1:A:1157:ILE:HD11	1.67	0.74
1:A:107:ASN:HB3	1:A:119:PHE:CZ	2.24	0.73
1:A:521:ARG:CG	1:A:521:ARG:HH11	2.01	0.73
1:A:1103:GLU:HG3	1:A:1104:PRO:HD2	1.73	0.70
1:A:841:HIS:O	1:A:842:ILE:HB	1.91	0.69
1:A:897:GLN:H	1:A:897:GLN:HE21	1.39	0.69
1:A:917:GLY:O	1:A:918:ARG:HB2	1.91	0.69
1:A:67:ARG:O	1:A:68:TYR:HB2	1.92	0.68
1:A:444:GLY:N	1:A:605:THR:HG22	1.96	0.68
3:A:1406:OSA:C5	3:A:1406:OSA:H30	2.26	0.66
1:A:967:ILE:HB	1:A:968:PRO:HD3	1.77	0.65
1:A:920:PHE:CD1	1:A:920:PHE:O	2.45	0.63
1:A:536:PHE:O	1:A:539:THR:HG22	1.99	0.63
1:A:1280:MET:O	1:A:1281:ASN:HB2	2.01	0.61
1:A:111:VAL:HG13	1:A:116:GLY:HA2	1.81	0.61
1:A:842:ILE:HA	1:A:845:PHE:HD2	1.66	0.60
1:A:939:ILE:O	1:A:943:GLU:HG2	2.02	0.59
1:A:731:GLU:O	1:A:732:GLU:HB2	2.01	0.59
1:A:449:LEU:HD23	1:A:623:ILE:HB	1.84	0.59
1:A:393:LEU:O	1:A:395:ARG:N	2.36	0.59
1:A:769:PRO:O	1:A:772:SER:HB3	2.03	0.59
1:A:106:ILE:HD11	1:A:779:MET:O	2.03	0.58
1:A:1073:LEU:O	1:A:1237:LYS:HG2	2.04	0.58
1:A:286:ARG:NH2	1:A:846:ASP:OD1	2.36	0.57
1:A:298:LEU:HD13	1:A:838:LEU:HD12	1.84	0.57
1:A:422:HIS:HB2	1:A:472:LYS:HB3	1.87	0.57
1:A:920:PHE:HD1	1:A:920:PHE:C	2.09	0.56
1:A:906:LEU:HB3	3:A:1405:OSA:H14	1.88	0.56
1:A:920:PHE:CD1	1:A:920:PHE:C	2.79	0.56
1:A:183:GLU:H	1:A:398:VAL:HG21	1.71	0.56
1:A:1174:ILE:HG22	1:A:1233:VAL:HG11	1.88	0.55
1:A:487:LEU:HD23	1:A:491:ARG:HH12	1.71	0.55
1:A:750:HIS:CE1	1:A:824:SER:HB3	2.41	0.55
1:A:771:TYR:HB2	1:A:803:LEU:HD21	1.89	0.54
1:A:623:ILE:HG12	1:A:633:VAL:HG22	1.90	0.54
1:A:1075:GLY:HA3	1:A:1268:THR:HG21	1.88	0.54
1:A:421:VAL:HG13	1:A:470:VAL:HG13	1.90	0.54
1:A:1173:ILE:HA	1:A:1230:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:GLN:NE2	1:A:353:GLY:H	2.06	0.53
1:A:613:LEU:H	1:A:653:GLN:HE22	1.56	0.52
1:A:119:PHE:O	1:A:123:GLY:HA2	2.10	0.52
1:A:418:VAL:HB	1:A:439:LEU:HG	1.92	0.51
1:A:1239:LEU:HD22	1:A:1241:LEU:HD12	1.92	0.51
1:A:776:THR:HG21	1:A:1019:ARG:HA	1.93	0.51
1:A:393:LEU:C	1:A:395:ARG:H	2.14	0.51
1:A:184:ILE:CG2	1:A:946:ARG:CZ	2.89	0.51
1:A:1257:GLN:HA	1:A:1260:LEU:HD12	1.92	0.50
1:A:863:VAL:HB	1:A:864:PRO:HD3	1.93	0.50
1:A:26:LYS:HG2	1:A:30:LYS:HE2	1.92	0.50
1:A:748:ARG:N	1:A:749:PRO:HD2	2.27	0.50
1:A:521:ARG:NH1	1:A:521:ARG:HG3	2.17	0.50
1:A:217:ALA:O	1:A:221:LEU:HB2	2.12	0.50
3:A:1406:OSA:H35	3:A:1406:OSA:H30	1.92	0.50
1:A:578:LEU:HD22	1:A:597:LEU:HD22	1.92	0.50
1:A:1199:PHE:O	1:A:1203:LEU:HB2	2.11	0.50
1:A:424:THR:HA	1:A:433:ILE:HD12	1.95	0.49
1:A:521:ARG:NH1	1:A:521:ARG:CG	2.68	0.49
2:A:1402:NAG:H3	2:A:1403:BMA:O5	2.12	0.49
2:A:1402:NAG:H5	2:A:1403:BMA:O2	2.13	0.49
1:A:516:LYS:HB2	1:A:570:VAL:HG12	1.95	0.48
1:A:186:TRP:CD1	1:A:396:LYS:HE2	2.48	0.48
1:A:910:ALA:HB2	3:A:1405:OSA:H19	1.95	0.48
1:A:651:THR:HA	1:A:654:THR:HG22	1.96	0.48
1:A:1076:LYS:HE2	1:A:1078:ILE:HD11	1.95	0.48
1:A:720:LYS:HG2	1:A:721:ASP:H	1.78	0.48
1:A:61:SER:HB3	1:A:63:PRO:HD2	1.96	0.48
1:A:1155:ILE:HG12	1:A:1238:ILE:HG12	1.95	0.48
1:A:491:ARG:HG2	1:A:950:ALA:HA	1.95	0.47
1:A:309:LYS:HD2	1:A:827:ARG:HE	1.80	0.47
1:A:327:GLN:HB3	1:A:807:GLN:HE21	1.79	0.47
1:A:358:THR:O	1:A:362:VAL:HG23	2.14	0.47
1:A:487:LEU:HD12	1:A:487:LEU:H	1.80	0.47
1:A:188:ASP:OD1	1:A:946:ARG:NH2	2.47	0.47
1:A:135:VAL:HG11	1:A:1002:LEU:HB2	1.96	0.47
1:A:1106:GLN:HE21	1:A:1283:ASP:HB3	1.80	0.47
1:A:1007:THR:O	1:A:1010:PRO:HB3	2.14	0.47
1:A:1004:LEU:HB3	1:A:1012:MET:HB2	1.95	0.47
1:A:762:THR:HG23	1:A:882:VAL:HG21	1.97	0.47
1:A:739:ASN:HD21	1:A:741:PHE:HB2	1.79	0.47
1:A:1075:GLY:CA	1:A:1268:THR:HG21	2.44	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:ASN:HB3	1:A:119:PHE:CE2	2.51	0.46
1:A:916:ARG:HH22	3:A:1406:OSA:H36	1.80	0.46
1:A:1146:LEU:HB3	1:A:1151:THR:HG21	1.97	0.46
1:A:1113:PRO:HG2	1:A:1116:CYS:HB3	1.98	0.46
1:A:455:CYS:SG	1:A:457:LYS:HD2	2.55	0.45
1:A:446:THR:HG23	1:A:606:THR:HB	1.99	0.45
1:A:782:PHE:HA	1:A:789:PHE:CE1	2.52	0.45
1:A:1177:LEU:H	1:A:1177:LEU:HD12	1.82	0.45
1:A:743:ILE:HG22	1:A:870:ILE:HD12	1.98	0.45
1:A:390:TYR:HA	1:A:393:LEU:HB3	1.98	0.44
1:A:777:SER:OG	1:A:1019:ARG:NH2	2.50	0.44
1:A:119:PHE:HB3	1:A:121:PRO:HD2	1.98	0.44
1:A:1085:ALA:H	1:A:1132:LEU:HD13	1.81	0.44
1:A:187:PHE:CZ	1:A:945:VAL:HG21	2.52	0.44
1:A:342:VAL:HG11	1:A:793:GLY:HA3	2.00	0.44
1:A:1031:LEU:CD2	3:A:1405:OSA:H16	2.47	0.44
1:A:435:ARG:HH21	1:A:627:ASN:HB3	1.83	0.44
1:A:1015:MET:O	1:A:1019:ARG:HG3	2.17	0.43
1:A:933:ASP:HB3	1:A:964:LYS:NZ	2.33	0.43
1:A:1253:GLU:O	1:A:1257:GLN:HB2	2.18	0.43
1:A:774:PHE:CE1	1:A:799:MET:HB3	2.54	0.43
1:A:62:ILE:N	1:A:63:PRO:CD	2.82	0.43
1:A:507:THR:HA	1:A:546:THR:O	2.19	0.43
1:A:839:SER:HB3	1:A:1064:LEU:HD12	2.00	0.43
1:A:822:SER:HB2	1:A:867:ARG:HG3	2.00	0.43
1:A:576:LEU:HD23	1:A:606:THR:HG23	2.01	0.43
1:A:101:VAL:HB	1:A:138:VAL:HG11	2.01	0.43
1:A:1018:LEU:HD23	1:A:1021:MET:HE1	2.00	0.43
1:A:782:PHE:HA	1:A:789:PHE:HE1	1.84	0.43
1:A:285:ILE:HA	1:A:288:VAL:HG12	2.00	0.43
1:A:1022:TYR:O	1:A:1026:ILE:HB	2.19	0.43
1:A:906:LEU:N	1:A:907:PRO:HD2	2.34	0.42
1:A:97:LEU:HD21	1:A:141:SER:HB3	2.01	0.42
1:A:910:ALA:HB1	3:A:1406:OSA:H12	2.01	0.42
1:A:742:GLU:O	1:A:746:HIS:HD2	2.02	0.42
1:A:863:VAL:HG22	1:A:1051:ILE:HD13	2.01	0.42
1:A:119:PHE:CE2	1:A:126:TYR:CG	3.07	0.42
1:A:514:LEU:HD22	1:A:953:ARG:HG2	2.01	0.42
1:A:562:ARG:HA	1:A:565:ILE:HD12	2.00	0.42
1:A:543:GLY:O	1:A:546:THR:HG22	2.19	0.42
1:A:1177:LEU:HD12	1:A:1234:ARG:NH1	2.35	0.41
1:A:111:VAL:HG23	1:A:119:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:VAL:HG13	1:A:222:SER:CB	2.51	0.41
1:A:184:ILE:HG21	1:A:946:ARG:NH1	2.36	0.41
1:A:1231:ALA:O	1:A:1236:PRO:HD3	2.20	0.41
1:A:420:ASN:H	1:A:438:ASN:ND2	2.18	0.41
1:A:613:LEU:O	1:A:616:ILE:HG22	2.21	0.41
1:A:396:LYS:HA	1:A:397:PRO:HD3	1.86	0.41
1:A:509:GLU:HB3	1:A:544:TYR:HB3	2.02	0.41
1:A:1182:VAL:HG21	1:A:1233:VAL:HG13	2.02	0.40
1:A:864:PRO:O	1:A:867:ARG:HB3	2.22	0.40
1:A:841:HIS:ND1	1:A:1060:LYS:HB2	2.36	0.40
1:A:85:VAL:HG13	1:A:222:SER:HB3	2.03	0.40
1:A:1038:PHE:N	1:A:1039:PRO:HD2	2.36	0.40
1:A:737:LYS:HA	1:A:1049:GLY:HA3	2.02	0.40
1:A:731:GLU:O	1:A:732:GLU:CB	2.69	0.40
1:A:1280:MET:O	1:A:1281:ASN:CB	2.69	0.40
1:A:888:ILE:HG23	1:A:903:ILE:HD11	2.04	0.40
1:A:5:GLY:HA2	1:A:8:ARG:HG2	2.02	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	1244/1321 (94%)	1175 (94%)	63 (5%)	6 (0%)	38 87

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ASP
1	A	842	ILE
1	A	735	ALA
1	A	393	LEU
1	A	871	ASP
1	A	1265	GLU

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	984/1099 (90%)	951 (97%)	33 (3%)	49 88

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	120	LEU
1	A	124	GLN
1	A	127	THR
1	A	191	HIS
1	A	221	LEU
1	A	286	ARG
1	A	356	LEU
1	A	400	ASP
1	A	428	ARG
1	A	430	ASP
1	A	457	LYS
1	A	465	LEU
1	A	496	VAL
1	A	521	ARG
1	A	576	LEU
1	A	621	LEU
1	A	780	ASN
1	A	841	HIS
1	A	842	ILE
1	A	870	ILE
1	A	897	GLN
1	A	918	ARG
1	A	920	PHE
1	A	923	LYS
1	A	924	ASN
1	A	965	LEU
1	A	1011	THR
1	A	1146	LEU
1	A	1238	ILE
1	A	1268	THR

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Mol	Chain	Res	Type
1	A	1303	MET
1	A	1305	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	191	HIS
1	A	249	GLN
1	A	330	ASN
1	A	383	GLN
1	A	438	ASN
1	A	486	ASN
1	A	554	GLN
1	A	739	ASN
1	A	746	HIS
1	A	750	HIS
1	A	780	ASN
1	A	807	GLN
1	A	831	ASN
1	A	840	GLN
1	A	897	GLN
1	A	949	GLN
1	A	1106	GLN
1	A	1172	ASN
1	A	1186	GLN
1	A	1301	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 carbohydrates 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	NDG	A	1401	1,2	12,14,15	1.00	1 (8%)	15,19,21	1.30	3 (20%)
2	NAG	A	1402	2	12,14,15	1.09	1 (8%)	15,19,21	1.20	1 (6%)
2	BMA	A	1403	2	10,11,12	0.91	0	11,15,17	0.79	0
2	MAN	A	1404	2	10,11,12	0.79	0	11,15,17	0.70	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
2	NDG	A	1401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1402	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1403	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1404	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1402	NAG	C3-C2	2.85	1.58	1.52
2	A	1401	NDG	O-C5	2.26	1.49	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	NDG	C3-C2-N2	-3.18	106.91	111.76
2	A	1401	NDG	O-C5-C4	2.58	113.93	110.65
2	A	1402	NAG	C3-C2-N2	-2.50	107.96	111.76
2	A	1401	NDG	O-C5-C6	2.47	109.57	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

2 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	OSA	A	1405	-	35,35,35	0.47	0	46,46,46	0.95	1 (2%)
3	OSA	A	1406	-	35,35,35	0.47	0	46,46,46	1.08	2 (4%)

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	OSA	A	1405	-	-	0/20/60/60	0/2/2/2
3	OSA	A	1406	-	-	1/20/60/60	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1406	OSA	CA-S1'-C1'	3.50	105.27	100.19
3	A	1406	OSA	O5'-C1'-S1'	-3.30	101.63	109.96
3	A	1405	OSA	O5'-C1'-C2'	-2.27	107.50	110.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1406	OSA	O5'-C1'-S1'-CA

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1250/1321 (94%)	0.15	13 (1%)	79 44	105, 140, 192, 200	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	GLU	3.4
1	A	1245	THR	2.6
1	A	1256	VAL	2.4
1	A	1296	LYS	2.3
1	A	1279	VAL	2.2
1	A	1204	PRO	2.2
1	A	1110	LEU	2.2
1	A	1295	GLU	2.1
1	A	1303	MET	2.1
1	A	921	THR	2.1
1	A	918	ARG	2.0
1	A	1092	ILE	2.0
1	A	1306	LYS	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 ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NDG	A	1401	14/15	0.38	5.03	195,199,200,200	0
2	BMA	A	1403	11/12	0.32	-	200,200,200,200	0
2	MAN	A	1404	11/12	0.33	-	191,200,200,200	0
2	NAG	A	1402	14/15	0.37	-	196,200,200,200	0

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. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	0SA	A	1406	34/34	0.51	3.24	134,190,198,198	0
3	0SA	A	1405	34/34	0.54	3.12	147,171,178,179	0

6.5 Other polymers

There are no such residues in this entry.