



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:33 pm GMT

PDB ID : 4F4C  
Title : The Crystal Structure of the Multi-Drug Transporter  
Authors : Jin, M.S.; Oldham, M.L.; Zhang, Q.; Chen, J.  
Deposited on : 2012-05-10  
Resolution : 3.40 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](mailto: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.

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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 : trunk28683  
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

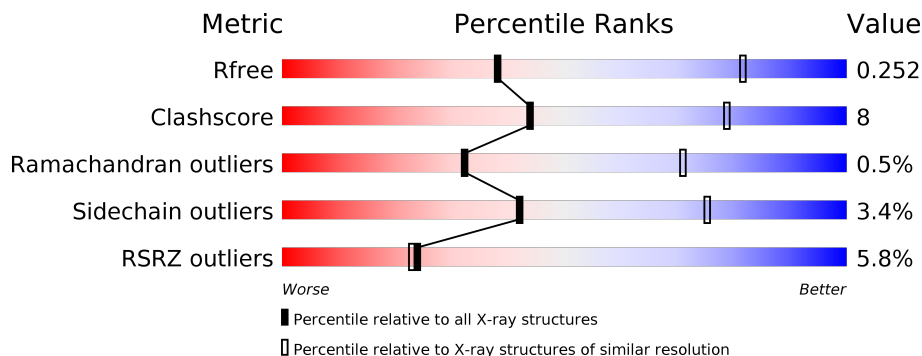
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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  $\geq 3$ , 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	1321	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 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.

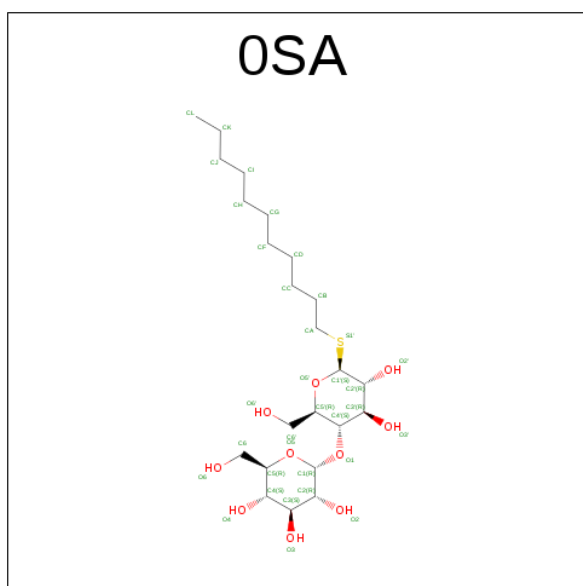
- Molecule 1 is a protein called Multidrug resistance protein pgp-1.

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: C<sub>23</sub>H<sub>44</sub>O<sub>10</sub>S).

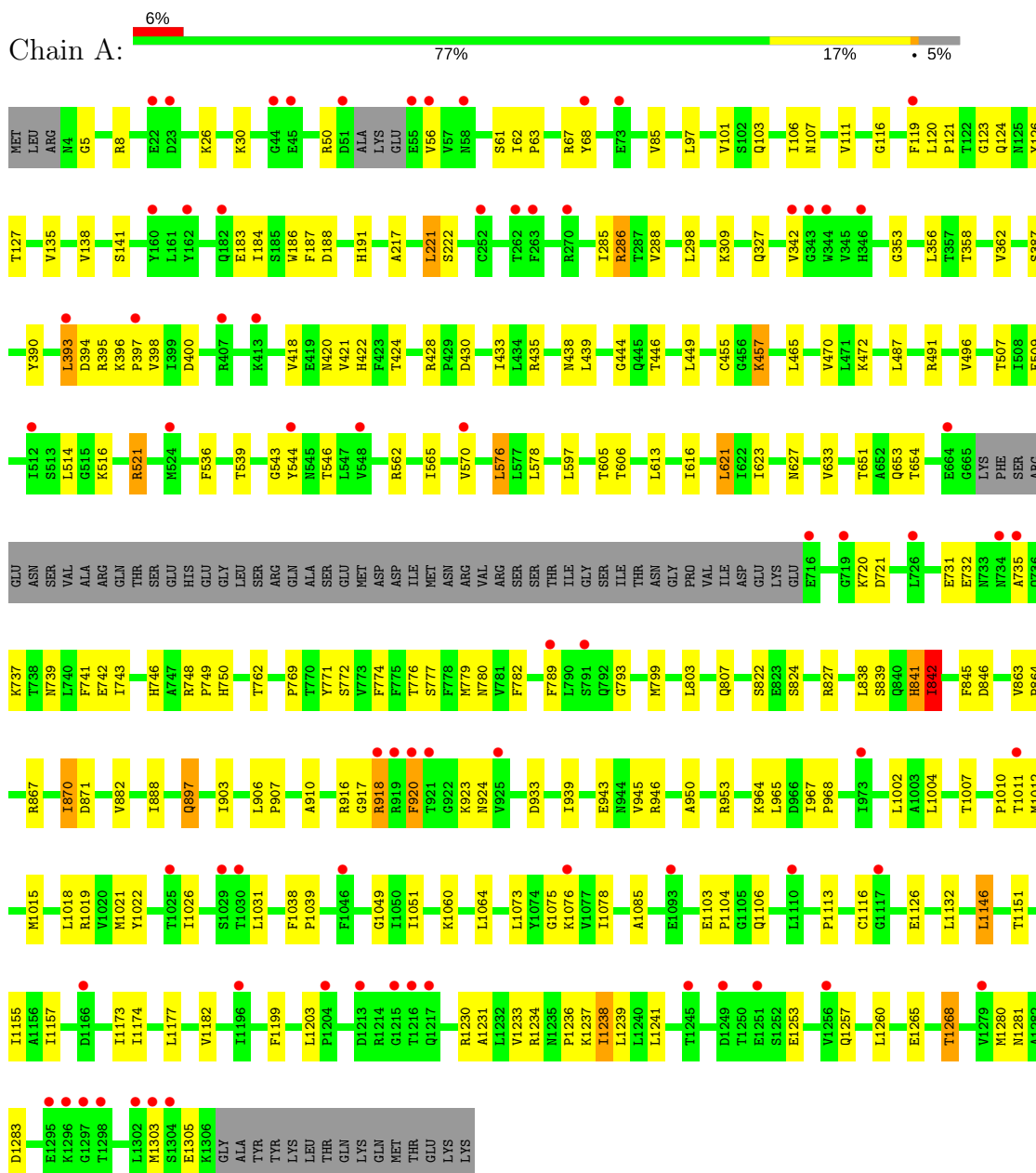


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			34	23	10	1		
3	A	1	Total	C	O	S	0	0
			34	23	10	1		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Multidrug resistance protein pgp-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.250 , 0.283 0.250 , 0.252	Depositor DCC
$R_{free}$ test set	1719 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	140.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 88.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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 8.

All (144) 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:444:GLY:H	1:A:605:THR:HG22	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:ILE:HA	1:A:1230:ARG:HG2	1.90	0.53
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:217:ALA:O	1:A:221:LEU:HB2	2.12	0.50
1:A:521:ARG:NH1	1:A:521:ARG:HG3	2.17	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:61:SER:HB3	1:A:63:PRO:HD2	1.96	0.48
1:A:720:LYS:HG2	1:A:721:ASP:H	1.78	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:135:VAL:HG11	1:A:1002:LEU:HB2	1.96	0.47
1:A:1007:THR:O	1:A:1010:PRO:HB3	2.14	0.47
1:A:1106:GLN:HE21	1:A:1283:ASP:HB3	1.80	0.47
1:A:487:LEU:H	1:A:487:LEU:HD12	1.80	0.47
1:A:188:ASP:OD1	1:A:946:ARG:NH2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:446:THR:HG23	1:A:606:THR:HB	1.99	0.45
1:A:455:CYS:SG	1:A:457:LYS:HD2	2.55	0.45
1:A:1177:LEU:H	1:A:1177:LEU:HD12	1.82	0.45
1:A:782:PHE:HA	1:A:789:PHE:CE1	2.52	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:1085:ALA:H	1:A:1132:LEU:HD13	1.81	0.44
1:A:119:PHE:HB3	1:A:121:PRO:HD2	1.98	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:839:SER:HB3	1:A:1064:LEU:HD12	2.00	0.43
1:A:507:THR:HA	1:A:546:THR:O	2.19	0.43
1:A:62:ILE:N	1:A:63:PRO:CD	2.82	0.43
1:A:822:SER:HB2	1:A:867:ARG:HG3	2.00	0.43
1:A:1018:LEU:HD23	1:A:1021:MET:HE1	2.00	0.43
1:A:101:VAL:HB	1:A:138:VAL:HG11	2.01	0.43
1:A:576:LEU:HD23	1:A:606:THR:HG23	2.01	0.43
1:A:1022:TYR:O	1:A:1026:ILE:HB	2.19	0.43
1:A:285:ILE:HA	1:A:288:VAL:HG12	2.00	0.43
1:A:782:PHE:HA	1:A:789:PHE:HE1	1.84	0.43
1:A:97:LEU:HD21	1:A:141:SER:HB3	2.01	0.42
1:A:906:LEU:N	1:A:907:PRO:HD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:85:VAL:HG13	1:A:222:SER:CB	2.51	0.41
1:A:1231:ALA:O	1:A:1236:PRO:HD3	2.20	0.41
1:A:184:ILE:HG21	1:A:946:ARG:NH1	2.36	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:1038:PHE:N	1:A:1039:PRO:HD2	2.36	0.40
1:A:841:HIS:ND1	1:A:1060:LYS:HB2	2.36	0.40
1:A:737:LYS:HA	1:A:1049:GLY:HA3	2.02	0.40
1:A:85:VAL:HG13	1:A:222:SER:HB3	2.03	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 [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	1244/1321 (94%)	1175 (94%)	63 (5%)	6 (0%)	32 71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ASP

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Mol	Chain	Res	Type
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%)	42 75

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

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Mol	Chain	Res	Type
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
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 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 ⓘ

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	14,14,15	1.41	3 (21%)	15,19,21	1.42	1 (6%)
2	NAG	A	1402	2	14,14,15	1.75	2 (14%)	15,19,21	1.29	2 (13%)
2	BMA	A	1403	2	11,11,12	1.18	1 (9%)	13,15,17	0.68	0
2	MAN	A	1404	2	11,11,12	1.14	1 (9%)	13,15,17	0.88	1 (7%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	NDG	C1-C2	2.20	1.55	1.52
2	A	1403	BMA	C2-C3	2.28	1.55	1.52
2	A	1401	NDG	O-C1	2.69	1.48	1.43
2	A	1404	MAN	C2-C3	2.73	1.56	1.52
2	A	1402	NAG	C3-C2	2.74	1.58	1.52
2	A	1401	NDG	O-C5	2.93	1.49	1.43
2	A	1402	NAG	C1-C2	5.29	1.59	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1402	NAG	C1-C2-N2	-2.08	106.94	110.49
2	A	1404	MAN	C1-O5-C5	2.19	115.18	112.17
2	A	1402	NAG	C4-C3-C2	2.69	114.96	111.02
2	A	1401	NDG	C1-O-C5	4.72	118.67	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1402	NAG	2	0
2	A	1403	BMA	2	0

## 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	0.49	0	45,46,46	0.93	1 (2%)
3	OSA	A	1406	-	35,35,35	0.48	0	45,46,46	1.10	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	O5'-C1'-S1'	-3.22	101.63	110.15
3	A	1405	OSA	O5'-C1'-C2'	-2.03	107.50	110.28
3	A	1406	OSA	CA-S1'-C1'	3.36	105.27	100.28

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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1405	OSA	3	0
3	A	1406	OSA	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1250/1321 (94%)	0.54	73 (5%) 24 23	105, 140, 192, 200	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	GLU	4.6
1	A	56	VAL	4.5
1	A	1256	VAL	4.5
1	A	119	PHE	4.5
1	A	1279	VAL	4.2
1	A	1296	LYS	3.9
1	A	920	PHE	3.7
1	A	1245	THR	3.6
1	A	1204	PRO	3.6
1	A	58	ASN	3.5
1	A	1298	THR	3.5
1	A	263	PHE	3.4
1	A	51	ASP	3.3
1	A	343	GLY	3.3
1	A	397	PRO	3.3
1	A	1295	GLU	3.3
1	A	68	TYR	3.2
1	A	921	THR	3.2
1	A	918	ARG	3.1
1	A	23	ASP	3.1
1	A	512	ILE	3.0
1	A	1025	THR	3.0
1	A	45	GLU	3.0
1	A	1251	GLU	2.9
1	A	413	LYS	2.9
1	A	524	MET	2.9
1	A	1029	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	789	PHE	2.8
1	A	1110	LEU	2.8
1	A	791	SER	2.8
1	A	1166	ASP	2.8
1	A	44	GLY	2.7
1	A	342	VAL	2.7
1	A	162	TYR	2.7
1	A	664	GLU	2.7
1	A	726	LEU	2.7
1	A	1117	GLY	2.6
1	A	1249	ASP	2.6
1	A	1196	ILE	2.6
1	A	1213	ASP	2.6
1	A	734	ASN	2.6
1	A	22	GLU	2.5
1	A	270	ARG	2.5
1	A	1030	THR	2.5
1	A	1046	PHE	2.5
1	A	719	GLY	2.5
1	A	1303	MET	2.5
1	A	1216	THR	2.5
1	A	973	ILE	2.4
1	A	544	TYR	2.4
1	A	1297	GLY	2.4
1	A	735	ALA	2.4
1	A	1302	LEU	2.3
1	A	262	THR	2.3
1	A	393	LEU	2.3
1	A	182	GLN	2.3
1	A	570	VAL	2.3
1	A	1011	THR	2.3
1	A	73	GLU	2.2
1	A	160	TYR	2.2
1	A	925	VAL	2.1
1	A	1217	GLN	2.1
1	A	344	TRP	2.1
1	A	1304	SER	2.1
1	A	55	GLU	2.1
1	A	346	HIS	2.1
1	A	548	VAL	2.1
1	A	252	CYS	2.0
1	A	407	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1093	GLU	2.0
1	A	1076	LYS	2.0
1	A	1215	GLY	2.0
1	A	919	ARG	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](#)

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	1402	14/15	0.55	0.53	-	196,200,200,200	0
2	BMA	A	1403	11/12	0.60	0.44	-	200,200,200,200	0
2	MAN	A	1404	11/12	0.58	0.51	-	191,200,200,200	0
2	NDG	A	1401	14/15	0.59	0.57	-	195,199,200,200	0

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	OSA	A	1406	34/34	0.56	0.52	2.74	134,190,198,198	0
3	OSA	A	1405	34/34	0.63	0.58	2.59	147,171,178,179	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.