



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:39 PM GMT

PDB ID : 1Q25  
Title : Crystal structure of N-terminal 3 domains of CI-MPR  
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Deposited on : 2003-07-23  
Resolution : 1.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

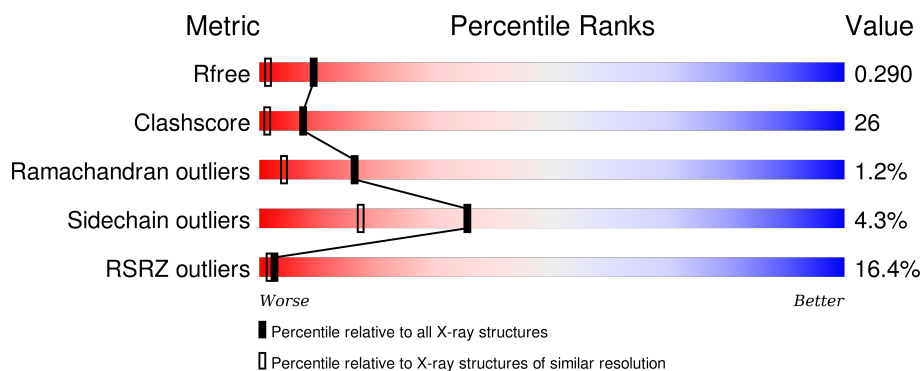
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	432	<div> <div>16%</div> <div>67%</div> <div>28%</div> <div>..</div> </div>

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	NAG	A	2001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	4005	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3763 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 cation-independent mannose 6-phosphate receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3303	2060	564	651	28			

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

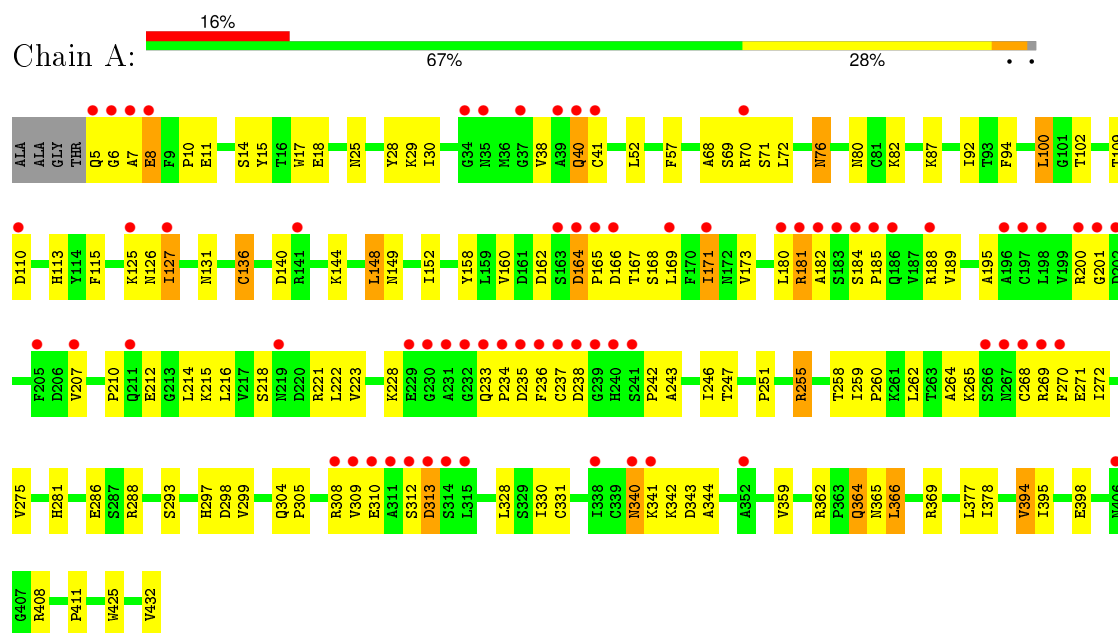
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	365	Total	O	0	0
			365	365		

### 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 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: cation-independent mannose 6-phosphate receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.16Å 84.75Å 96.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 1.80 19.94 – 1.75	Depositor EDS
% Data completeness (in resolution range)	87.1 (19.94-1.80) 81.9 (19.94-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 1.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.235 , 0.283 0.245 , 0.290	Depositor DCC
$R_{free}$ test set	2820 reflections (6.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 41940 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, 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	0.36	1/3371 (0.0%)	0.67	1/4570 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	GLU	CD-OE2	7.52	1.33	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ASN	CB-CA-C	-6.43	97.54	110.40

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	3303	0	3159	170	0
2	A	61	0	52	1	0
3	A	28	0	25	2	0
4	A	6	0	4	0	0
5	A	365	0	0	11	0
All	All	3763	0	3240	170	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 26.

All (170) 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:92:ILE:HD13	1:A:115:PHE:HB2	1.37	1.04
1:A:246:ILE:HD13	1:A:272:ILE:HB	1.49	0.94
1:A:309:VAL:HG11	1:A:313:ASP:OD1	1.71	0.91
1:A:228:LYS:HB3	1:A:228:LYS:HZ2	1.33	0.90
1:A:164:ASP:HB3	1:A:167:THR:OG1	1.73	0.88
1:A:378:ILE:CD1	1:A:394:VAL:HB	2.04	0.88
1:A:80:ASN:HD21	1:A:87:LYS:HZ3	1.22	0.87
1:A:109:THR:HG22	1:A:110:ASP:H	1.43	0.84
1:A:293:SER:H	1:A:297:HIS:HD2	1.24	0.84
1:A:195:ALA:HB2	1:A:210:PRO:HD3	1.57	0.84
1:A:149:ASN:HA	1:A:152:ILE:HD13	1.59	0.84
1:A:309:VAL:HG13	1:A:408:ARG:NH2	1.94	0.81
1:A:76:ASN:OD1	5:A:774:HOH:O	1.99	0.79
1:A:80:ASN:HD21	1:A:87:LYS:NZ	1.81	0.77
1:A:207:VAL:HG23	1:A:242:PRO:HB3	1.67	0.76
1:A:299:VAL:HG23	1:A:432:VAL:HG13	1.68	0.75
1:A:92:ILE:HD13	1:A:115:PHE:CB	2.16	0.74
1:A:160:VAL:CG2	1:A:171:ILE:HD12	2.18	0.73
1:A:228:LYS:HB3	1:A:228:LYS:NZ	2.03	0.73
1:A:185:PRO:HA	1:A:188:ARG:HE	1.53	0.72
1:A:309:VAL:CG1	1:A:313:ASP:OD1	2.36	0.72
1:A:236:PHE:CE1	1:A:237:CYS:SG	2.82	0.72
1:A:6:GLY:HA2	1:A:10:PRO:CG	2.21	0.70
1:A:80:ASN:ND2	1:A:87:LYS:NZ	2.40	0.70
1:A:14:SER:HB2	1:A:15:TYR:CE1	2.27	0.69
1:A:330:ILE:HG23	1:A:331:CYS:SG	2.31	0.69
1:A:109:THR:HG22	1:A:110:ASP:N	2.07	0.69
1:A:242:PRO:HA	1:A:268:CYS:O	1.93	0.68
1:A:40:GLN:H	1:A:40:GLN:NE2	1.92	0.68
1:A:246:ILE:CD1	1:A:272:ILE:HB	2.21	0.68
1:A:184:SER:O	1:A:188:ARG:HG3	1.94	0.68
1:A:40:GLN:H	1:A:40:GLN:HE21	1.40	0.68
1:A:215:LYS:HE2	1:A:223:VAL:HG23	1.76	0.68
1:A:411:PRO:HG3	1:A:425:TRP:CZ3	2.29	0.67
1:A:340:ASN:CG	1:A:341:LYS:H	1.97	0.67
1:A:149:ASN:CA	1:A:152:ILE:HD13	2.25	0.66
1:A:25:ASN:ND2	1:A:52:LEU:HB2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLN:H	1:A:364:GLN:NE2	1.94	0.65
1:A:364:GLN:H	1:A:364:GLN:HE21	1.44	0.65
1:A:233:GLN:HG3	1:A:242:PRO:HD3	1.79	0.64
1:A:160:VAL:HG23	1:A:171:ILE:HD12	1.77	0.64
1:A:251:PRO:HG3	1:A:275:VAL:CG1	2.28	0.63
1:A:136:CYS:SG	1:A:152:ILE:HD11	2.39	0.62
1:A:341:LYS:C	1:A:341:LYS:HD3	2.21	0.61
1:A:378:ILE:HD13	1:A:394:VAL:HB	1.80	0.61
1:A:242:PRO:HG3	1:A:268:CYS:SG	2.40	0.61
1:A:125:LYS:C	1:A:127:ILE:H	2.04	0.60
1:A:242:PRO:HA	1:A:268:CYS:HB3	1.84	0.60
1:A:233:GLN:HG3	1:A:242:PRO:CD	2.32	0.59
1:A:411:PRO:HG3	1:A:425:TRP:CE3	2.36	0.59
1:A:207:VAL:O	1:A:207:VAL:HG22	2.03	0.59
1:A:11:GLU:HG3	5:A:697:HOH:O	2.02	0.58
1:A:340:ASN:ND2	1:A:341:LYS:H	2.00	0.58
1:A:71:SER:HB2	1:A:94:PHE:O	2.04	0.58
1:A:207:VAL:HG21	1:A:270:PHE:CE1	2.39	0.58
1:A:341:LYS:HD3	1:A:341:LYS:O	2.04	0.57
1:A:28:TYR:OH	1:A:113:HIS:HD2	1.88	0.57
1:A:341:LYS:O	1:A:343:ASP:N	2.36	0.57
1:A:265:LYS:NZ	1:A:265:LYS:HB3	2.20	0.57
1:A:127:ILE:HD13	1:A:127:ILE:O	2.05	0.56
1:A:6:GLY:HA2	1:A:10:PRO:HG2	1.87	0.56
1:A:246:ILE:HD11	1:A:272:ILE:HD12	1.88	0.56
1:A:182:ALA:HB3	1:A:188:ARG:HG2	1.87	0.56
1:A:378:ILE:HD12	1:A:394:VAL:HB	1.89	0.55
1:A:299:VAL:HG23	1:A:432:VAL:CG1	2.36	0.55
1:A:286:GLU:OE1	1:A:369:ARG:HD3	2.06	0.55
1:A:259:ILE:HG23	1:A:260:PRO:HD2	1.89	0.55
1:A:171:ILE:H	1:A:171:ILE:HD13	1.72	0.55
1:A:158:TYR:HB2	1:A:171:ILE:CD1	2.37	0.55
1:A:364:GLN:O	1:A:365:ASN:OD1	2.24	0.55
1:A:164:ASP:CB	1:A:167:THR:OG1	2.53	0.54
1:A:82:LYS:HD3	1:A:110:ASP:OD1	2.07	0.54
1:A:309:VAL:HG12	1:A:310:GLU:N	2.22	0.54
1:A:218:SER:OG	1:A:221:ARG:HB2	2.07	0.54
1:A:125:LYS:O	1:A:127:ILE:N	2.41	0.54
1:A:180:LEU:HB2	1:A:181:ARG:HD2	1.89	0.54
1:A:181:ARG:N	1:A:181:ARG:HD2	2.23	0.54
1:A:243:ALA:HB2	1:A:269:ARG:NH1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:H	1:A:11:GLU:CD	2.12	0.53
1:A:166:ASP:O	1:A:200:ARG:HA	2.08	0.53
1:A:362:ARG:HD3	5:A:844:HOH:O	2.08	0.53
1:A:158:TYR:O	1:A:171:ILE:HD13	2.08	0.53
1:A:365:ASN:OD1	3:A:2001:NAG:H2	2.09	0.53
1:A:125:LYS:C	1:A:127:ILE:N	2.61	0.53
1:A:288:ARG:HG2	5:A:672:HOH:O	2.09	0.53
1:A:5:GLN:HE21	1:A:5:GLN:HA	1.74	0.52
1:A:144:LYS:HG3	1:A:281:HIS:HD2	1.74	0.52
1:A:365:ASN:OD1	3:A:2001:NAG:C2	2.57	0.52
1:A:6:GLY:HA2	1:A:10:PRO:HG3	1.91	0.51
1:A:140:ASP:OD2	1:A:144:LYS:HB2	2.10	0.51
1:A:243:ALA:N	1:A:268:CYS:O	2.43	0.51
1:A:264:ALA:HB3	1:A:271:GLU:HB2	1.92	0.51
1:A:304:GLN:N	1:A:305:PRO:HD2	2.26	0.51
1:A:251:PRO:HG2	1:A:255:ARG:HD2	1.92	0.51
1:A:148:LEU:O	1:A:152:ILE:CD1	2.59	0.50
1:A:5:GLN:NE2	1:A:5:GLN:HA	2.26	0.50
1:A:5:GLN:HG3	1:A:6:GLY:N	2.26	0.50
1:A:246:ILE:CD1	1:A:272:ILE:HD12	2.42	0.49
1:A:207:VAL:CG2	1:A:242:PRO:HB3	2.40	0.49
1:A:395:ILE:HD12	1:A:395:ILE:N	2.27	0.49
1:A:127:ILE:HD13	1:A:127:ILE:C	2.33	0.49
1:A:76:ASN:HB3	5:A:644:HOH:O	2.12	0.48
1:A:200:ARG:O	1:A:200:ARG:HG2	2.14	0.48
1:A:72:LEU:HD12	1:A:92:ILE:O	2.13	0.48
1:A:80:ASN:ND2	1:A:87:LYS:HZ2	2.12	0.48
1:A:364:GLN:C	1:A:365:ASN:OD1	2.52	0.48
1:A:251:PRO:HG3	1:A:275:VAL:HG12	1.93	0.48
1:A:343:ASP:HA	5:A:925:HOH:O	2.13	0.48
1:A:340:ASN:CG	1:A:341:LYS:N	2.67	0.48
1:A:125:LYS:HB2	1:A:127:ILE:HG22	1.96	0.48
1:A:309:VAL:HG13	1:A:408:ARG:HH21	1.76	0.48
1:A:215:LYS:HE2	1:A:223:VAL:CG2	2.44	0.47
1:A:40:GLN:HB3	1:A:57:PHE:HB2	1.96	0.47
1:A:237:CYS:O	1:A:238:ASP:HB2	2.14	0.47
1:A:234:PRO:O	1:A:235:ASP:HB2	2.13	0.47
1:A:152:ILE:N	1:A:152:ILE:HD12	2.30	0.47
1:A:432:VAL:HG12	1:A:432:VAL:OXT	2.14	0.47
1:A:366:LEU:C	1:A:366:LEU:HD12	2.35	0.47
1:A:259:ILE:CG2	1:A:260:PRO:HD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:OE2	1:A:68:ALA:CB	2.64	0.46
1:A:5:GLN:HG3	1:A:7:ALA:H	1.80	0.46
1:A:214:LEU:HD21	1:A:222:LEU:HD13	1.98	0.46
1:A:286:GLU:O	1:A:297:HIS:HE1	1.98	0.46
1:A:158:TYR:HB2	1:A:171:ILE:HD11	1.97	0.46
1:A:152:ILE:HG13	1:A:173:VAL:O	2.16	0.46
1:A:109:THR:CG2	1:A:110:ASP:N	2.78	0.45
1:A:233:GLN:CG	1:A:242:PRO:HD3	2.47	0.45
1:A:30:ILE:N	1:A:30:ILE:HD12	2.30	0.45
1:A:243:ALA:HB3	1:A:269:ARG:HD2	1.99	0.45
1:A:255:ARG:NH2	1:A:258:THR:OG1	2.50	0.45
1:A:18:GLU:HA	1:A:28:TYR:O	2.17	0.44
1:A:265:LYS:NZ	1:A:265:LYS:CB	2.80	0.44
1:A:131:ASN:HB2	5:A:762:HOH:O	2.16	0.44
1:A:6:GLY:CA	1:A:10:PRO:HG3	2.48	0.44
1:A:70:ARG:NH1	5:A:855:HOH:O	2.49	0.44
1:A:305:PRO:O	1:A:308:ARG:HG2	2.18	0.44
1:A:293:SER:H	1:A:297:HIS:CD2	2.16	0.44
1:A:181:ARG:N	1:A:181:ARG:CD	2.81	0.44
1:A:109:THR:CG2	1:A:110:ASP:H	2.22	0.43
1:A:158:TYR:HB2	1:A:171:ILE:HD13	2.00	0.43
1:A:265:LYS:HB3	1:A:265:LYS:HZ3	1.84	0.43
1:A:69:SER:HB2	1:A:72:LEU:HB3	1.99	0.43
1:A:270:PHE:H	1:A:270:PHE:HD1	1.65	0.43
1:A:76:ASN:OD1	2:A:1001:NAG:C2	2.67	0.43
1:A:432:VAL:CG1	1:A:432:VAL:OXT	2.67	0.43
1:A:270:PHE:N	1:A:270:PHE:CD1	2.87	0.43
1:A:221:ARG:NH1	1:A:247:THR:HG21	2.33	0.42
1:A:185:PRO:HA	1:A:188:ARG:NE	2.29	0.42
1:A:17:TRP:HH2	1:A:100:LEU:HD13	1.85	0.42
1:A:6:GLY:C	1:A:10:PRO:HG3	2.39	0.42
1:A:310:GLU:O	1:A:312:SER:N	2.47	0.42
1:A:293:SER:N	1:A:297:HIS:HD2	2.05	0.42
1:A:297:HIS:O	1:A:298:ASP:HB2	2.20	0.42
1:A:160:VAL:HG22	1:A:171:ILE:HD12	1.97	0.42
1:A:366:LEU:HD13	1:A:377:LEU:HD11	2.01	0.42
1:A:340:ASN:CB	5:A:790:HOH:O	2.68	0.41
1:A:216:LEU:HD23	1:A:216:LEU:C	2.41	0.41
1:A:189:VAL:O	1:A:189:VAL:HG12	2.20	0.41
1:A:164:ASP:HA	1:A:165:PRO:HD3	1.88	0.41
1:A:10:PRO:HD2	1:A:11:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:N	5:A:925:HOH:O	2.53	0.41
1:A:162:ASP:HB3	1:A:262:LEU:HD12	2.02	0.41
1:A:92:ILE:HD13	1:A:115:PHE:CG	2.55	0.41
1:A:344:ALA:HB2	1:A:359:VAL:HG22	2.03	0.41
1:A:38:VAL:HB	1:A:41:CYS:SG	2.60	0.41
1:A:29:LYS:C	1:A:30:ILE:HD12	2.41	0.41
1:A:102:THR:HG23	5:A:635:HOH:O	2.20	0.41
1:A:182:ALA:O	1:A:188:ARG:HD3	2.21	0.40
1:A:378:ILE:HD13	1:A:394:VAL:HA	2.04	0.40
1:A:328:LEU:N	1:A:328:LEU:HD12	2.37	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	426/432 (99%)	392 (92%)	29 (7%)	5 (1%)	16 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	342	LYS
1	A	201	GLY
1	A	126	ASN
1	A	8	GLU

### 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	368/370 (100%)	352 (96%)	16 (4%)	35	17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	100	LEU
1	A	127	ILE
1	A	136	CYS
1	A	148	LEU
1	A	164	ASP
1	A	168	SER
1	A	169	LEU
1	A	171	ILE
1	A	181	ARG
1	A	255	ARG
1	A	313	ASP
1	A	364	GLN
1	A	366	LEU
1	A	394	VAL
1	A	398	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	24	ASN
1	A	25	ASN
1	A	40	GLN
1	A	58	HIS
1	A	80	ASN
1	A	85	ASN
1	A	113	HIS
1	A	149	ASN
1	A	233	GLN
1	A	297	HIS
1	A	304	GLN
1	A	348	GLN

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Mol	Chain	Res	Type
1	A	364	GLN
1	A	401	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 ⓘ

7 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	NAG	A	1001	1,2	14,14,15	1.31	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	A	1002	2	14,14,15	0.53	0	15,19,21	0.95	0
2	MAN	A	1003	2	11,11,12	0.42	0	14,15,17	0.64	0
2	MAN	A	1004	2	11,11,12	0.49	0	14,15,17	0.53	0
2	BMA	A	1005	2	11,11,12	0.57	0	14,15,17	0.42	0
3	NAG	A	2001	1,3	14,14,15	0.99	1 (7%)	15,19,21	1.03	2 (13%)
3	NAG	A	2002	3	14,14,15	0.56	0	15,19,21	0.79	1 (6%)

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	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	MAN	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
2	BMA	A	1005	2	-	0/2/19/22	0/1/1/1
3	NAG	A	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2002	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	NAG	C4-C5	2.02	1.57	1.53
2	A	1001	NAG	C4-C3	2.33	1.58	1.52
2	A	1001	NAG	C1-C2	3.40	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	NAG	C2-N2-C7	-2.24	120.16	123.04
2	A	1001	NAG	C2-N2-C7	-2.19	120.22	123.04
3	A	2001	NAG	C2-N2-C7	-2.11	120.33	123.04
3	A	2001	NAG	C3-C4-C5	2.36	114.32	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	1	0
3	A	2001	NAG	2	0

## 5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z  > 2$
4	GOL	A	4005	-	5,5,5	4.89	5 (100%)	5,5,5	5.66	3 (60%)

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
4	GOL	A	4005	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4005	GOL	C3-C2	-8.30	1.20	1.52
4	A	4005	GOL	C1-C2	-3.25	1.39	1.52
4	A	4005	GOL	O2-C2	-2.85	1.35	1.43
4	A	4005	GOL	O3-C3	3.37	1.56	1.42
4	A	4005	GOL	O1-C1	4.57	1.62	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4005	GOL	O1-C1-C2	3.18	125.59	110.18
4	A	4005	GOL	O2-C2-C3	6.59	138.86	108.65
4	A	4005	GOL	O3-C3-C2	10.31	160.18	110.18

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 ⓘ

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, 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	428/432 (99%)	0.85	70 (16%) 2 2	13, 28, 68, 83	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	CYS	8.6
1	A	166	ASP	8.2
1	A	236	PHE	8.0
1	A	341	LYS	7.9
1	A	5	GLN	7.4
1	A	315	LEU	7.0
1	A	311	ALA	6.8
1	A	6	GLY	6.8
1	A	340	ASN	6.3
1	A	163	SER	6.3
1	A	237	CYS	6.2
1	A	309	VAL	6.1
1	A	312	SER	5.9
1	A	7	ALA	5.8
1	A	238	ASP	5.3
1	A	165	PRO	5.3
1	A	180	LEU	4.7
1	A	181	ARG	4.7
1	A	127	ILE	4.6
1	A	240	HIS	4.6
1	A	185	PRO	4.3
1	A	266	SER	4.3
1	A	269	ARG	4.2
1	A	310	GLU	4.1
1	A	183	SER	4.1
1	A	202	ASP	4.1
1	A	235	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	182	ALA	4.0
1	A	34	GLY	3.8
1	A	267	ASN	3.8
1	A	229	GLU	3.7
1	A	205	PHE	3.4
1	A	200	ARG	3.4
1	A	201	GLY	3.4
1	A	164	ASP	3.4
1	A	232	GLY	3.3
1	A	125	LYS	3.3
1	A	234	PRO	3.1
1	A	219	ASN	3.0
1	A	233	GLN	3.0
1	A	313	ASP	3.0
1	A	35	ASN	2.9
1	A	40	GLN	2.8
1	A	70	ARG	2.8
1	A	39	ALA	2.7
1	A	230	GLY	2.7
1	A	186	GLN	2.7
1	A	8	GLU	2.7
1	A	188	ARG	2.7
1	A	239	GLY	2.7
1	A	241	SER	2.7
1	A	231	ALA	2.6
1	A	314	SER	2.6
1	A	141	ARG	2.5
1	A	308	ARG	2.5
1	A	270	PHE	2.4
1	A	41	CYS	2.4
1	A	406	ASN	2.4
1	A	207	VAL	2.4
1	A	196	ALA	2.4
1	A	184	SER	2.3
1	A	198	LEU	2.3
1	A	197	CYS	2.3
1	A	171	ILE	2.2
1	A	110	ASP	2.2
1	A	37	GLY	2.1
1	A	211	GLN	2.1
1	A	338	ILE	2.0
1	A	169	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	352	ALA	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
3	NAG	A	2001	14/15	0.73	0.29	3.02	47,51,55,57	0
2	NAG	A	1001	14/15	0.84	0.15	0.59	27,30,32,33	0
2	MAN	A	1004	11/12	0.86	0.13	0.09	19,21,25,31	0
2	NAG	A	1002	14/15	0.86	0.15	-	30,33,37,39	0
2	MAN	A	1003	11/12	0.82	0.23	-	40,42,45,47	0
3	NAG	A	2002	14/15	0.56	0.44	-	60,62,63,64	0
2	BMA	A	1005	11/12	0.91	0.12	-	22,27,31,36	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
4	GOL	A	4005	6/6	0.84	0.16	-	36,39,41,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.