



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:17 PM GMT

PDB ID : 1SZ0  
Title : N-terminal 3 domains of CI-MPR bound to mannose 6-phosphate  
Authors : Olson, L.J.; Dahms, N.M.; Kim, J.-J.P.  
Deposited on : 2004-04-01  
Resolution : 2.10 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

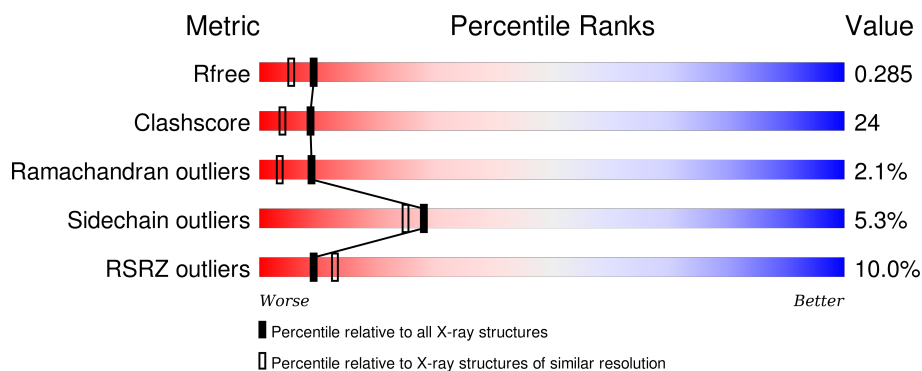
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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>12%</div> <div>57%</div> <div>35%</div> <div>.</div> <div>.</div> </div>
1	B	432	<div> <div>8%</div> <div>59%</div> <div>34%</div> <div>.</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	B	1501	-	-	-	X
3	NAG	B	1601	-	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6811 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	417	Total	C	N	O	S	0	0	0
			3218	2011	546	633	28			
1	B	416	Total	C	N	O	S	0	0	0
			3219	2014	548	629	28			

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

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

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

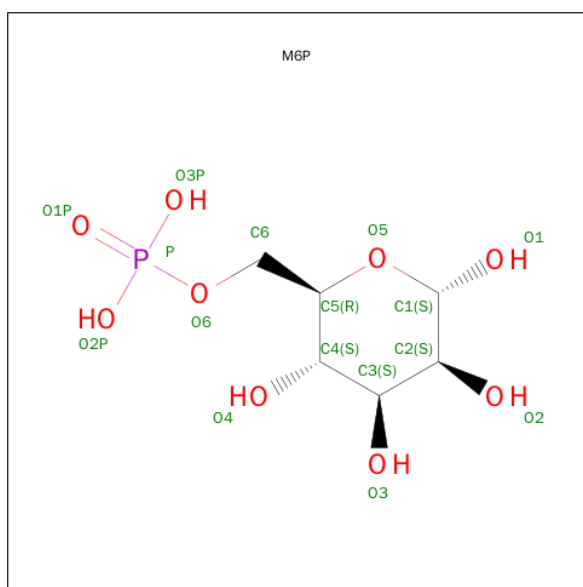


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is OSMIUM ION (three-letter code: OS) (formula: Os).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Os	0	0
			1	1		
5	A	1	Total	Os	0	0
			1	1		

- Molecule 6 is ALPHA-D-MANNOSE-6-PHOSPHATE (three-letter code: M6P) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			16	6	9	1		
6	B	1	Total	C	O	P	0	0
			16	6	9	1		

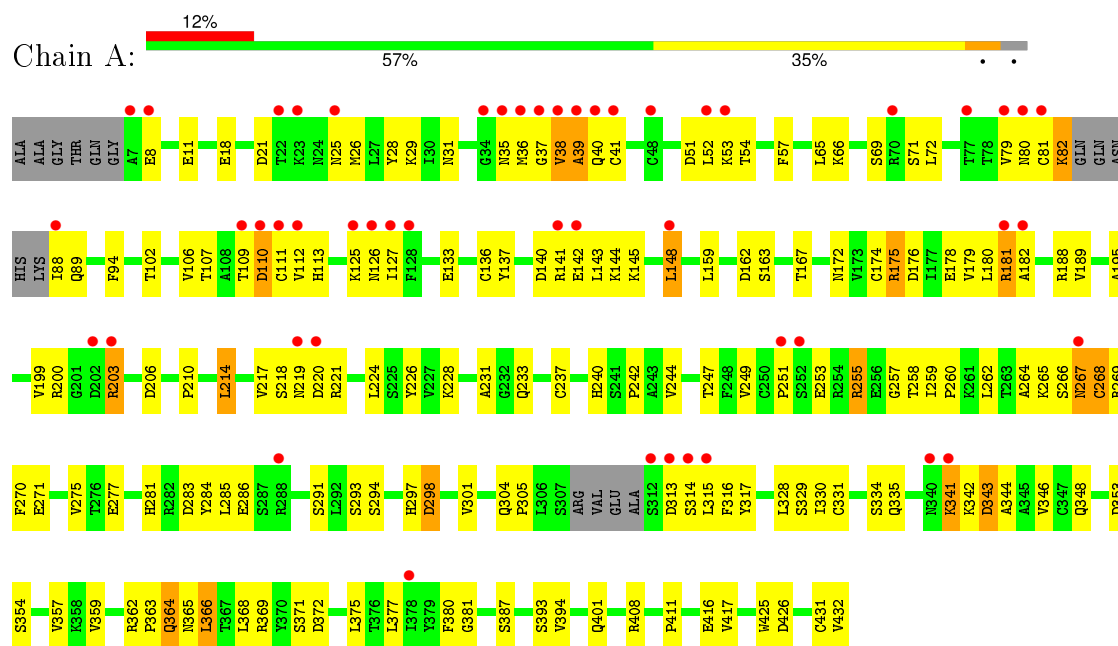
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	97	Total	O	0	0
			97	97		
7	B	145	Total	O	0	0
			145	145		

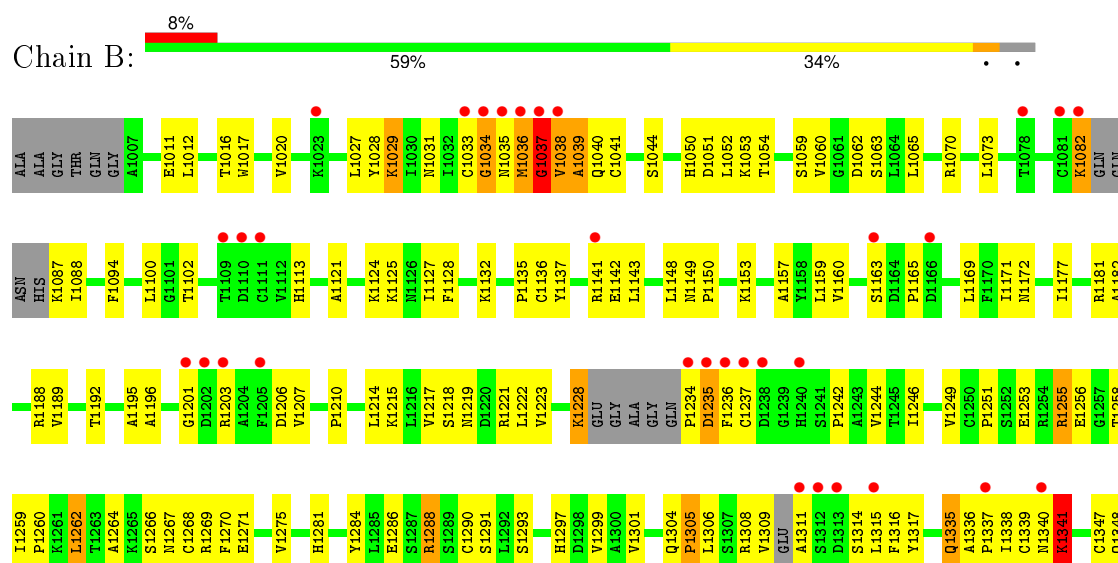
### 3 Residue-property plots

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: cation-independent mannose 6-phosphate receptor



- Molecule 1: cation-independent mannose 6-phosphate receptor







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.10 Å   86.50 Å   84.80 Å 90.00°   109.57°   90.00°	Depositor
Resolution (Å)	28.80 – 2.10 28.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (28.80-2.10) 81.1 (28.80-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.00 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.238 , 0.287 0.236 , 0.285	Depositor DCC
$R_{free}$ test set	2993 reflections (6.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.4	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46471 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6811	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M6P, OS, NAG, NDG

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	0.40	0/3283	0.68	3/4450 (0.1%)
1	B	0.44	3/3283 (0.1%)	0.76	10/4447 (0.2%)
All	All	0.42	3/6566 (0.0%)	0.72	13/8897 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1036	MET	N-CA	-5.46	1.35	1.46
1	B	1037	GLY	N-CA	-5.05	1.38	1.46
1	B	1038	VAL	CA-CB	-5.03	1.44	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1036	MET	CA-C-N	-12.61	90.97	116.20
1	B	1037	GLY	CA-C-N	-10.14	94.89	117.20
1	B	1036	MET	O-C-N	8.21	137.16	123.20
1	B	1038	VAL	N-CA-C	-7.74	90.10	111.00
1	B	1038	VAL	N-CA-CB	7.63	128.29	111.50
1	A	203	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	A	343	ASP	N-CA-CB	7.25	123.64	110.60
1	B	1036	MET	N-CA-C	6.38	128.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1036	MET	C-N-CA	6.31	135.56	122.30
1	B	1038	VAL	CA-CB-CG1	-6.29	101.46	110.90
1	B	1036	MET	CA-C-O	5.42	131.48	120.10
1	B	1037	GLY	O-C-N	5.15	130.95	122.70
1	A	237	CYS	CA-CB-SG	-5.07	104.87	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1037	GLY	Mainchain

## 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	3218	0	3084	160	0
1	B	3219	0	3098	130	0
2	A	28	0	25	3	0
3	B	56	0	50	18	0
4	A	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	16	0	11	1	0
6	B	16	0	11	1	0
7	A	97	0	0	2	0
7	B	145	0	0	6	0
All	All	6811	0	6292	303	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 24.

All (303) 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:267:ASN:HD21	1:A:269:ARG:CG	1.73	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:HG23	1:A:218:SER:H	1.24	0.99
3:B:1501:NAG:H5	3:B:1502:NAG:H2	1.42	0.97
1:B:1365:ASN:HD21	3:B:1601:NAG:C7	1.78	0.97
1:A:342:LYS:NZ	1:A:362:ARG:HH22	1.60	0.97
1:A:221:ARG:HH11	1:A:247:THR:HG21	1.31	0.95
1:B:1365:ASN:HD21	3:B:1601:NAG:C2	1.80	0.94
1:B:1020:VAL:HG12	1:B:1027:LEU:HD13	1.52	0.92
1:A:266:SER:O	1:A:267:ASN:ND2	2.03	0.92
1:A:267:ASN:HD21	1:A:269:ARG:HG3	1.36	0.91
1:A:106:VAL:HG23	1:A:107:THR:HG22	1.52	0.90
1:B:1218:SER:HB3	1:B:1221:ARG:HB2	1.54	0.90
1:B:1365:ASN:ND2	3:B:1601:NAG:N2	2.19	0.89
1:A:342:LYS:HZ3	1:A:362:ARG:HH22	1.13	0.88
1:B:1299:VAL:HG23	1:B:1432:VAL:HG13	1.57	0.86
1:B:1207:VAL:HG23	1:B:1242:PRO:HB3	1.57	0.85
1:A:40:GLN:HB3	1:A:57:PHE:HB2	1.61	0.83
1:B:1011:GLU:HG3	7:B:5070:HOH:O	1.78	0.82
1:A:267:ASN:ND2	1:A:269:ARG:CG	2.42	0.82
3:B:1501:NAG:H5	3:B:1502:NAG:C2	2.10	0.81
1:A:221:ARG:HH11	1:A:247:THR:CG2	1.94	0.79
1:B:1125:LYS:HE3	7:B:5152:HOH:O	1.82	0.79
1:B:1038:VAL:O	1:B:1040:GLN:N	2.17	0.78
1:A:148:LEU:HD22	1:A:214:LEU:HD11	1.66	0.77
1:A:25:ASN:ND2	1:A:52:LEU:HB2	1.98	0.77
1:A:364:GLN:H	1:A:364:GLN:NE2	1.82	0.77
1:A:328:LEU:HD22	1:A:346:VAL:HG22	1.68	0.74
1:A:285:LEU:HD22	1:A:371:SER:HB2	1.68	0.74
1:A:293:SER:H	1:A:297:HIS:HD2	1.33	0.74
1:A:25:ASN:HD21	1:A:52:LEU:HB2	1.50	0.74
1:B:1308:ARG:HA	1:B:1315:LEU:HD22	1.68	0.74
2:A:501:NDG:H4	2:A:502:NAG:N2	2.03	0.73
1:A:88:ILE:HG12	1:A:111:CYS:HB3	1.71	0.73
3:B:1501:NAG:H3	3:B:1502:NAG:O5	1.89	0.73
1:B:1053:LYS:HE3	1:B:1054:THR:HG23	1.69	0.73
1:B:1195:ALA:HB2	1:B:1210:PRO:HD3	1.70	0.73
1:B:1365:ASN:ND2	3:B:1601:NAG:C2	2.48	0.72
1:A:304:GLN:N	1:A:305:PRO:HD2	2.04	0.72
1:B:1365:ASN:ND2	3:B:1601:NAG:C7	2.51	0.72
1:B:1163:SER:O	1:B:1165:PRO:HD3	1.90	0.72
1:B:1214:LEU:HD11	1:B:1222:LEU:HD22	1.72	0.71
1:B:1363:PRO:HG2	1:B:1364:GLN:NE2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HA	1:A:111:CYS:O	1.91	0.71
1:A:264:ALA:HB3	1:A:271:GLU:HB2	1.70	0.71
1:A:267:ASN:C	1:A:267:ASN:HD22	1.92	0.70
3:B:1601:NAG:H61	3:B:1602:NAG:H82	1.73	0.70
1:A:195:ALA:HB2	1:A:210:PRO:HD3	1.72	0.70
1:A:175:ARG:HG2	1:A:176:ASP:N	2.07	0.69
1:A:411:PRO:HG3	1:A:425:TRP:CZ3	2.28	0.69
1:A:365:ASN:HD22	1:A:381:GLY:HA3	1.58	0.69
1:B:1127:ILE:HG23	1:B:1128:PHE:HD1	1.58	0.69
1:A:411:PRO:HG3	1:A:425:TRP:CE3	2.28	0.68
1:A:259:ILE:HG23	1:A:260:PRO:HD2	1.73	0.68
1:B:1020:VAL:HG12	1:B:1027:LEU:CD1	2.22	0.68
1:B:1207:VAL:HG21	1:B:1270:PHE:CE1	2.28	0.68
1:A:217:VAL:HG23	1:A:218:SER:N	2.03	0.68
1:B:1251:PRO:HG3	1:B:1255:ARG:HD2	1.76	0.68
1:A:35:ASN:HB2	7:A:5144:HOH:O	1.93	0.67
1:B:1335:GLN:CD	1:B:1336:ALA:H	1.97	0.67
1:B:1242:PRO:HA	1:B:1268:CYS:O	1.94	0.67
1:B:1206:ASP:OD1	1:B:1228:LYS:HD3	1.95	0.67
1:B:1293:SER:H	1:B:1297:HIS:HD2	1.42	0.66
1:A:8:GLU:HG3	1:A:66:LYS:NZ	2.11	0.66
1:A:341:LYS:HE3	1:A:342:LYS:HB2	1.77	0.66
1:B:1366:LEU:HG	1:B:1377:LEU:HD11	1.78	0.65
1:A:221:ARG:NH1	1:A:247:THR:HG21	2.08	0.64
1:B:1038:VAL:C	1:B:1040:GLN:H	2.00	0.64
1:B:1038:VAL:C	1:B:1040:GLN:N	2.50	0.63
1:A:267:ASN:ND2	1:A:269:ARG:HG2	2.13	0.63
1:B:1259:ILE:HG23	1:B:1260:PRO:HD2	1.81	0.63
1:B:1286:GLU:OE1	1:B:1369:ARG:HD3	1.99	0.63
1:A:267:ASN:O	1:A:267:ASN:ND2	2.31	0.63
1:A:218:SER:HB3	1:A:221:ARG:CB	2.29	0.63
1:A:36:MET:SD	1:A:38:VAL:HG22	2.39	0.63
1:B:1365:ASN:HD21	3:B:1601:NAG:H2	1.65	0.62
1:B:1033:CYS:O	1:B:1035:ASN:N	2.34	0.61
1:A:218:SER:HB3	1:A:221:ARG:HB3	1.81	0.61
1:B:1341:LYS:N	1:B:1341:LYS:HD3	2.16	0.61
1:A:38:VAL:O	1:A:38:VAL:HG23	2.01	0.60
1:A:21:ASP:HB3	1:A:26:MET:HB2	1.83	0.60
1:B:1264:ALA:HB3	1:B:1271:GLU:HB2	1.83	0.59
1:A:267:ASN:HD21	1:A:269:ARG:CB	2.15	0.59
1:B:1365:ASN:ND2	3:B:1601:NAG:O7	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:VAL:O	1:B:1207:VAL:HG22	2.02	0.59
1:B:1359:VAL:HB	1:B:1383:GLU:HG3	1.85	0.59
1:B:1182:ALA:HB3	1:B:1188:ARG:HG3	1.84	0.59
3:B:1502:NAG:O3	3:B:1502:NAG:H83	2.03	0.59
1:B:1037:GLY:HA2	1:B:1039:ALA:H	1.68	0.59
1:B:1012:LEU:HD21	1:B:1100:LEU:HD22	1.83	0.59
1:B:1214:LEU:HD11	1:B:1222:LEU:HB3	1.84	0.58
1:B:1288:ARG:HB3	1:B:1288:ARG:HH21	1.67	0.58
1:A:343:ASP:OD1	1:A:343:ASP:C	2.42	0.58
1:B:1157:ALA:HB1	1:B:1171:ILE:O	2.03	0.58
1:A:365:ASN:HB3	1:A:380:PHE:CD1	2.38	0.58
1:B:1127:ILE:HG23	1:B:1128:PHE:CD1	2.39	0.57
1:A:341:LYS:HD3	1:A:341:LYS:H	1.68	0.57
1:A:233:GLN:NE2	1:A:240:HIS:O	2.36	0.57
1:A:343:ASP:OD1	1:A:363:PRO:CD	2.53	0.57
1:B:1217:VAL:HG23	1:B:1218:SER:H	1.68	0.57
1:B:1337:PRO:HA	1:B:1340:ASN:CG	2.25	0.57
1:B:1051:ASP:OD1	1:B:1053:LYS:HB3	2.05	0.56
1:A:69:SER:OG	1:A:72:LEU:HB3	2.06	0.56
1:B:1309:VAL:HG22	1:B:1317:TYR:CE1	2.41	0.56
1:A:8:GLU:HG3	1:A:66:LYS:HZ1	1.69	0.56
1:B:1217:VAL:HG23	1:B:1218:SER:N	2.20	0.56
1:A:329:SER:CB	1:A:335:GLN:HE21	2.19	0.56
1:A:218:SER:O	1:A:220:ASP:N	2.38	0.56
1:B:1256:GLU:HG2	7:B:5087:HOH:O	2.06	0.56
1:A:218:SER:C	1:A:220:ASP:H	2.09	0.56
1:A:133:GLU:HG3	1:A:175:ARG:HB2	1.87	0.56
1:A:31:ASN:ND2	1:A:35:ASN:N	2.54	0.56
1:A:249:VAL:CG2	1:A:275:VAL:HG22	2.36	0.56
1:B:1141:ARG:HH21	1:B:1219:ASN:ND2	2.05	0.55
1:A:416:GLU:HG2	1:A:417:VAL:N	2.22	0.55
1:A:257:GLY:HA3	1:A:372:ASP:HB3	1.87	0.55
1:B:1028:TYR:OH	1:B:1113:HIS:HD2	1.89	0.55
1:A:344:ALA:HB2	1:A:359:VAL:HG13	1.88	0.55
1:B:1338:ILE:HG23	1:B:1339:CYS:SG	2.46	0.54
1:B:1016:THR:CG2	1:B:1029:LYS:HG3	2.38	0.54
1:A:71:SER:HB3	1:A:94:PHE:O	2.08	0.54
1:A:109:THR:OG1	1:A:112:VAL:HB	2.07	0.54
1:B:1359:VAL:HG23	1:B:1383:GLU:OE2	2.08	0.54
1:A:28:TYR:OH	1:A:113:HIS:HD2	1.91	0.54
1:B:1337:PRO:HA	1:B:1340:ASN:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:C	1:A:366:LEU:HD12	2.28	0.54
1:A:79:VAL:HG12	1:A:80:ASN:N	2.22	0.54
1:A:253:GLU:O	1:A:255:ARG:HG3	2.08	0.54
1:B:1366:LEU:HD23	1:B:1366:LEU:C	2.27	0.54
1:A:217:VAL:HG23	1:A:221:ARG:HB3	1.91	0.53
1:A:316:PHE:HB3	1:A:334:SER:O	2.08	0.53
1:A:140:ASP:OD2	1:A:144:LYS:HB2	2.09	0.53
1:B:1259:ILE:HD12	1:B:1259:ILE:N	2.23	0.53
2:A:501:NDG:H4	2:A:502:NAG:HN2	1.73	0.53
1:B:1304:GLN:N	1:B:1305:PRO:HD2	2.24	0.53
1:A:255:ARG:HH21	1:A:258:THR:HG23	1.73	0.53
1:A:343:ASP:OD1	1:A:363:PRO:HD2	2.08	0.53
1:A:174:CYS:H	1:A:224:LEU:HD21	1.74	0.53
1:A:162:ASP:O	1:A:163:SER:HB2	2.08	0.53
1:A:342:LYS:HZ3	1:A:362:ARG:NH2	1.96	0.52
1:B:1172:ASN:HB2	1:B:1177:ILE:HG12	1.92	0.52
1:B:1214:LEU:HD13	1:B:1215:LYS:N	2.24	0.52
1:B:1215:LYS:HE3	1:B:1223:VAL:HG23	1.92	0.52
1:B:1012:LEU:CD2	1:B:1100:LEU:HD22	2.40	0.52
1:A:255:ARG:NH2	1:A:258:THR:OG1	2.42	0.52
3:B:1501:NAG:H61	3:B:1502:NAG:O7	2.09	0.52
3:B:1601:NAG:C6	3:B:1602:NAG:H82	2.40	0.52
1:B:1266:SER:O	1:B:1269:ARG:HB3	2.09	0.52
1:A:281:HIS:CE1	1:A:284:TYR:HB2	2.45	0.52
1:A:408:ARG:HH11	1:A:408:ARG:HB3	1.76	0.51
1:B:1338:ILE:O	1:B:1341:LYS:HE2	2.11	0.51
1:A:51:ASP:OD1	1:A:53:LYS:HG2	2.10	0.51
3:B:1601:NAG:H5	3:B:1602:NAG:H82	1.92	0.51
1:A:341:LYS:HD3	1:A:341:LYS:N	2.25	0.51
1:B:1234:PRO:HB2	1:B:1237:CYS:SG	2.51	0.51
1:A:179:VAL:HG23	1:A:180:LEU:N	2.25	0.51
1:B:1304:GLN:C	1:B:1306:LEU:H	2.14	0.51
1:A:125:LYS:C	1:A:127:ILE:H	2.14	0.51
1:A:304:GLN:N	1:A:305:PRO:CD	2.73	0.51
1:B:1262:LEU:HD23	1:B:1271:GLU:O	2.11	0.51
1:B:1365:ASN:ND2	3:B:1601:NAG:H2	2.22	0.51
1:A:342:LYS:HZ1	1:A:362:ARG:HH22	1.52	0.51
1:A:36:MET:SD	1:A:38:VAL:CG2	3.00	0.50
1:B:1070:ARG:NH2	1:B:1124:LYS:HE3	2.26	0.50
1:A:267:ASN:ND2	1:A:269:ARG:HG3	2.12	0.50
1:A:145:LYS:O	1:A:281:HIS:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:THR:HG22	1:B:1137:TYR:CD2	2.46	0.50
1:A:40:GLN:HB3	1:A:57:PHE:CB	2.39	0.50
1:A:39:ALA:O	1:A:40:GLN:HB2	2.12	0.50
1:A:89:GLN:HG2	1:A:112:VAL:HG22	1.94	0.50
1:A:199:VAL:HA	1:A:203:ARG:O	2.11	0.50
1:A:218:SER:C	1:A:220:ASP:N	2.65	0.50
1:A:366:LEU:HD13	1:A:377:LEU:HD11	1.93	0.50
1:B:1380:PHE:HB2	7:B:5275:HOH:O	2.10	0.50
1:B:1311:ALA:N	1:B:1315:LEU:HD21	2.27	0.49
1:A:365:ASN:ND2	1:A:381:GLY:HA3	2.27	0.49
1:B:1041:CYS:HB3	1:B:1059:SER:HB2	1.93	0.49
1:A:365:ASN:HB3	1:A:380:PHE:CE1	2.47	0.49
1:A:18:GLU:OE2	1:A:29:LYS:HE2	2.11	0.49
1:A:342:LYS:NZ	1:A:362:ARG:NH2	2.44	0.49
1:A:65:LEU:HD12	1:A:65:LEU:N	2.27	0.49
1:B:1132:LYS:CG	1:B:1210:PRO:HG2	2.43	0.49
1:A:329:SER:HB3	1:A:335:GLN:HE21	1.78	0.49
1:B:1262:LEU:HD22	1:B:1264:ALA:H	1.78	0.48
1:B:1288:ARG:HB3	1:B:1288:ARG:NH2	2.28	0.48
1:B:1142:GLU:O	1:B:1143:LEU:HB2	2.13	0.48
1:B:1364:GLN:H	1:B:1364:GLN:CD	2.17	0.48
1:B:1291:SER:HB2	1:B:1301:VAL:O	2.14	0.48
1:A:189:VAL:O	1:A:189:VAL:HG12	2.14	0.48
1:B:1020:VAL:CG1	1:B:1027:LEU:HD13	2.34	0.48
1:A:364:GLN:HE21	1:A:364:GLN:H	1.58	0.48
1:A:109:THR:O	1:A:111:CYS:N	2.45	0.48
1:B:1065:LEU:N	1:B:1065:LEU:HD12	2.28	0.48
1:B:1215:LYS:HE3	1:B:1223:VAL:CG2	2.44	0.48
1:B:1034:GLY:HA3	1:B:1063:SER:OG	2.14	0.48
1:B:1304:GLN:O	1:B:1306:LEU:N	2.46	0.48
1:B:1249:VAL:HG13	1:B:1275:VAL:HA	1.95	0.48
1:B:1214:LEU:CD1	1:B:1222:LEU:HD22	2.40	0.48
1:A:242:PRO:HA	1:A:268:CYS:O	2.14	0.47
1:B:1073:LEU:HB2	1:B:1094:PHE:HE1	1.79	0.47
1:A:125:LYS:HD2	1:A:387:SER:HA	1.96	0.47
1:A:284:TYR:HE1	1:A:298:ASP:HB2	1.80	0.47
2:A:501:NDG:C4	2:A:502:NAG:N2	2.74	0.47
1:A:167:THR:HG21	1:A:200:ARG:HE	1.78	0.47
1:B:1401:GLN:HA	1:B:1401:GLN:NE2	2.30	0.47
1:B:1159:LEU:HD23	1:B:1160:VAL:N	2.29	0.47
1:A:291:SER:HA	1:A:301:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1011:GLU:HG2	1:B:1121:ALA:HB2	1.97	0.47
1:B:1256:GLU:HB3	7:B:5191:HOH:O	2.14	0.47
1:B:1281:HIS:CE1	1:B:1284:TYR:HB2	2.51	0.46
1:B:1050:HIS:O	1:B:1052:LEU:HD12	2.14	0.46
1:B:1038:VAL:O	1:B:1039:ALA:C	2.54	0.46
1:A:182:ALA:O	1:A:188:ARG:HD2	2.14	0.46
1:A:172:ASN:HB3	1:A:175:ARG:O	2.15	0.46
1:B:1347:CYS:SG	1:B:1357:VAL:HG13	2.54	0.46
1:B:1237:CYS:SG	1:B:1242:PRO:HG3	2.56	0.46
1:A:330:ILE:HG23	1:A:331:CYS:SG	2.56	0.46
1:A:267:ASN:O	1:A:268:CYS:CB	2.61	0.46
1:B:1290:CYS:SG	1:B:1366:LEU:HD11	2.56	0.46
1:A:125:LYS:O	1:A:127:ILE:N	2.45	0.46
1:A:255:ARG:NH2	1:A:258:THR:HG23	2.31	0.46
1:A:251:PRO:HG2	1:A:277:GLU:HG2	1.97	0.46
1:B:1314:SER:HB2	1:B:1316:PHE:CE1	2.51	0.46
1:A:206:ASP:O	1:A:228:LYS:HG3	2.17	0.45
1:A:51:ASP:OD1	1:A:54:THR:HG23	2.17	0.45
3:B:1601:NAG:H61	3:B:1602:NAG:C8	2.43	0.45
1:A:52:LEU:HD11	1:A:143:LEU:HD21	1.98	0.45
1:A:255:ARG:HH21	1:A:258:THR:CG2	2.29	0.45
1:A:102:THR:HG22	1:A:137:TYR:CD2	2.52	0.45
1:A:226:TYR:HB2	1:A:244:VAL:HB	1.98	0.45
1:B:1149:ASN:N	1:B:1150:PRO:CD	2.79	0.45
1:A:342:LYS:HD2	1:A:343:ASP:H	1.82	0.45
1:A:286:GLU:O	1:A:297:HIS:HE1	2.00	0.45
1:B:1418:ASP:O	1:B:1419:CYS:HB2	2.15	0.45
1:A:8:GLU:HG3	1:A:66:LYS:HZ2	1.82	0.45
1:A:217:VAL:CG2	1:A:218:SER:H	2.09	0.45
1:A:368:LEU:HD11	1:A:375:LEU:HD11	1.98	0.44
1:A:313:ASP:OD1	1:A:314:SER:N	2.50	0.44
1:B:1035:ASN:OD1	1:B:1036:MET:HG2	2.16	0.44
1:A:270:PHE:CD1	1:A:270:PHE:N	2.85	0.44
1:B:1201:GLY:O	1:B:1203:ARG:HG3	2.18	0.44
1:B:1196:ALA:CB	1:B:1244:VAL:HG21	2.48	0.44
1:A:251:PRO:CG	1:A:255:ARG:HD2	2.47	0.44
1:A:362:ARG:HH11	1:A:362:ARG:HG2	1.83	0.43
1:A:57:PHE:N	1:A:57:PHE:CD1	2.86	0.43
1:A:82:LYS:HD2	1:A:82:LYS:C	2.39	0.43
1:B:1011:GLU:CG	1:B:1121:ALA:HB2	2.47	0.43
1:B:1288:ARG:CB	1:B:1288:ARG:HH21	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:LYS:HE3	1:B:1054:THR:CG2	2.46	0.43
1:A:181:ARG:N	1:A:181:ARG:HD3	2.33	0.43
1:A:341:LYS:HE2	1:A:357:VAL:HG11	2.00	0.43
1:B:1314:SER:C	1:B:1316:PHE:H	2.22	0.43
1:A:218:SER:HB3	1:A:221:ARG:HB2	1.97	0.43
3:B:1601:NAG:C5	3:B:1602:NAG:H82	2.48	0.43
1:B:1223:VAL:HA	1:B:1246:ILE:O	2.18	0.43
1:B:1153:LYS:HD2	1:B:1157:ALA:HA	1.99	0.43
1:A:251:PRO:CB	1:A:255:ARG:HD2	2.49	0.43
1:B:1353:ASP:O	1:B:1355:THR:N	2.52	0.43
1:B:1235:ASP:O	1:B:1237:CYS:N	2.52	0.43
1:B:1141:ARG:HH21	1:B:1219:ASN:HD22	1.66	0.43
1:A:431:CYS:O	1:A:432:VAL:C	2.58	0.43
1:B:1382:GLY:O	1:B:1390:GLN:HG2	2.19	0.42
1:A:82:LYS:HE3	1:A:110:ASP:HB3	2.00	0.42
1:A:294:SER:O	1:A:298:ASP:HA	2.19	0.42
1:B:1411:PRO:HB3	1:B:1425:TRP:CE3	2.55	0.42
1:A:267:ASN:HD21	1:A:269:ARG:HB2	1.83	0.42
1:A:259:ILE:CG2	1:A:260:PRO:HD2	2.47	0.42
1:B:1255:ARG:HH21	1:B:1258:THR:HG23	1.84	0.42
1:A:262:LEU:HD11	1:A:265:LYS:HB2	2.01	0.42
1:B:1207:VAL:CG2	1:B:1242:PRO:HB3	2.39	0.42
1:A:11:GLU:HG3	7:A:5040:HOH:O	2.18	0.42
1:A:317:TYR:CD2	1:A:411:PRO:HD3	2.55	0.42
1:A:315:LEU:N	1:A:315:LEU:HD12	2.35	0.42
1:A:257:GLY:CA	1:A:372:ASP:HB3	2.50	0.42
1:B:1082:LYS:N	1:B:1082:LYS:HE3	2.35	0.42
1:B:1366:LEU:HD23	1:B:1367:THR:N	2.35	0.42
1:A:79:VAL:HG12	1:A:80:ASN:H	1.83	0.42
1:A:401:GLN:HA	1:A:401:GLN:HE21	1.85	0.42
1:A:18:GLU:HA	1:A:28:TYR:O	2.20	0.41
1:B:1087:LYS:HE2	7:B:5170:HOH:O	2.20	0.41
1:A:285:LEU:O	1:A:369:ARG:HA	2.20	0.41
1:B:1353:ASP:C	1:B:1355:THR:H	2.23	0.41
1:A:344:ALA:CB	1:A:359:VAL:HG13	2.49	0.41
1:A:142:GLU:O	1:A:143:LEU:HB2	2.20	0.41
1:A:346:VAL:HG21	1:A:393:SER:CB	2.51	0.41
1:A:281:HIS:NE2	1:A:284:TYR:HB2	2.36	0.41
1:A:37:GLY:O	1:A:38:VAL:C	2.59	0.41
1:A:267:ASN:ND2	1:A:269:ARG:CB	2.81	0.41
1:A:110:ASP:O	1:A:111:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1348:GLN:HE22	6:B:1500:M6P:C2	2.34	0.41
1:B:1011:GLU:CD	1:B:1011:GLU:H	2.24	0.41
1:B:1017:TRP:CH2	1:B:1135:PRO:HG3	2.56	0.41
1:B:1060:VAL:HG12	1:B:1088:ILE:HG21	2.02	0.41
1:B:1335:GLN:OE1	1:B:1339:CYS:HB2	2.21	0.41
1:A:416:GLU:CG	1:A:417:VAL:N	2.84	0.41
1:A:281:HIS:O	1:A:284:TYR:HB3	2.21	0.41
1:B:1044:SER:HB2	1:B:1062:ASP:OD1	2.21	0.41
1:A:343:ASP:O	1:A:362:ARG:NH1	2.54	0.41
1:A:113:HIS:ND1	1:A:113:HIS:N	2.69	0.40
1:A:89:GLN:HG3	1:A:112:VAL:HG13	2.04	0.40
1:A:348:GLN:HE22	6:A:500:M6P:C2	2.34	0.40
1:B:1189:VAL:HG12	1:B:1189:VAL:O	2.22	0.40
1:B:1207:VAL:HG21	1:B:1270:PHE:HE1	1.82	0.40
1:A:38:VAL:CG2	1:A:38:VAL:O	2.69	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	411/432 (95%)	361 (88%)	41 (10%)	9 (2%)	8	3
1	B	408/432 (94%)	371 (91%)	29 (7%)	8 (2%)	9	4
All	All	819/864 (95%)	732 (89%)	70 (8%)	17 (2%)	9	3

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ALA
1	B	1034	GLY
1	B	1235	ASP

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Mol	Chain	Res	Type
1	A	38	VAL
1	A	126	ASN
1	A	219	ASN
1	A	354	SER
1	B	1039	ALA
1	B	1236	PHE
1	B	1354	SER
1	A	81	CYS
1	A	110	ASP
1	B	1341	LYS
1	B	1267	ASN
1	B	1305	PRO
1	A	231	ALA
1	A	353	ASP

### 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	360/370 (97%)	340 (94%)	20 (6%)	26	22
1	B	361/370 (98%)	343 (95%)	18 (5%)	30	27
All	All	721/740 (97%)	683 (95%)	38 (5%)	28	25

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	CYS
1	A	82	LYS
1	A	136	CYS
1	A	141	ARG
1	A	148	LEU
1	A	159	LEU
1	A	175	ARG
1	A	178	GLU
1	A	181	ARG

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	255	ARG
1	A	267	ASN
1	A	268	CYS
1	A	283	ASP
1	A	298	ASP
1	A	341	LYS
1	A	364	GLN
1	A	366	LEU
1	A	394	VAL
1	A	426	ASP
1	B	1029	LYS
1	B	1031	ASN
1	B	1082	LYS
1	B	1136	CYS
1	B	1148	LEU
1	B	1169	LEU
1	B	1181	ARG
1	B	1192	THR
1	B	1228	LYS
1	B	1253	GLU
1	B	1255	ARG
1	B	1262	LEU
1	B	1288	ARG
1	B	1335	GLN
1	B	1341	LYS
1	B	1366	LEU
1	B	1394	VAL
1	B	1398	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	31	ASN
1	A	58	HIS
1	A	80	ASN
1	A	113	HIS
1	A	149	ASN
1	A	186	GLN
1	A	219	ASN
1	A	233	GLN

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Mol	Chain	Res	Type
1	A	240	HIS
1	A	267	ASN
1	A	297	HIS
1	A	304	GLN
1	A	335	GLN
1	A	348	GLN
1	A	364	GLN
1	A	401	GLN
1	B	1113	HIS
1	B	1126	ASN
1	B	1149	ASN
1	B	1219	ASN
1	B	1297	HIS
1	B	1304	GLN
1	B	1348	GLN
1	B	1365	ASN
1	B	1401	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 ⓘ

6 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	501	1,2	14,14,15	0.58	0	15,19,21	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	502	2	14,14,15	0.54	0	15,19,21	0.71	1 (6%)
3	NAG	B	1501	1,3	14,14,15	0.85	0	15,19,21	1.19	2 (13%)
3	NAG	B	1502	3	14,14,15	0.62	0	15,19,21	0.72	1 (6%)
3	NAG	B	1601	1,3	14,14,15	0.64	0	15,19,21	1.01	1 (6%)
3	NAG	B	1602	3	14,14,15	0.43	0	15,19,21	0.81	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	NDG	A	501	1,2	-	1/6/23/26	0/1/1/1
2	NAG	A	502	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1501	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	1502	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1602	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NDG	C2-N2-C7	-2.68	119.60	123.04
3	B	1601	NAG	C2-N2-C7	-2.43	119.92	123.04
3	B	1501	NAG	C2-N2-C7	-2.35	120.02	123.04
3	B	1602	NAG	C2-N2-C7	-2.20	120.22	123.04
3	B	1502	NAG	C2-N2-C7	-2.06	120.39	123.04
2	A	502	NAG	C2-N2-C7	-2.04	120.42	123.04
3	B	1501	NAG	C3-C4-C5	3.45	116.21	110.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	NAG	O7-C7-N2-C2
2	A	501	NDG	O7-C7-N2-C2
3	B	1501	NAG	O7-C7-N2-C2
3	B	1501	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDG	3	0
2	A	502	NAG	3	0
3	B	1501	NAG	4	0
3	B	1502	NAG	5	0
3	B	1601	NAG	13	0
3	B	1602	NAG	5	0

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	M6P	A	500	-	16,16,16	1.63	3 (18%)	23,24,24	0.83	0
4	NAG	A	601	1	14,14,15	0.59	0	15,19,21	0.75	1 (6%)
6	M6P	B	1500	-	16,16,16	1.59	3 (18%)	23,24,24	0.85	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
6	M6P	A	500	-	-	0/6/26/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
6	M6P	B	1500	-	-	0/6/26/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	500	M6P	C3-C2	2.17	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1500	M6P	C3-C2	2.23	1.58	1.52
6	B	1500	M6P	O5-C1	2.56	1.47	1.43
6	A	500	M6P	O5-C1	2.74	1.48	1.43
6	A	500	M6P	P-O1P	3.26	1.61	1.51
6	B	1500	M6P	P-O1P	3.43	1.62	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C2-N2-C7	-2.32	120.06	123.04

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
6	A	500	M6P	1	0
6	B	1500	M6P	1	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	417/432 (96%)	0.71	50 (11%) 6 8	22, 47, 74, 92	0
1	B	416/432 (96%)	0.53	33 (7%) 15 21	17, 39, 76, 93	0
All	All	833/864 (96%)	0.62	83 (9%) 9 13	17, 43, 75, 93	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1037	GLY	13.7
1	B	1313	ASP	9.5
1	B	1038	VAL	8.9
1	A	7	ALA	8.5
1	A	37	GLY	7.4
1	B	1340	ASN	5.8
1	A	40	GLN	5.6
1	B	1110	ASP	5.4
1	B	1237	CYS	5.4
1	B	1236	PHE	5.4
1	B	1201	GLY	5.3
1	A	25	ASN	5.3
1	A	219	ASN	5.2
1	A	312	SER	4.8
1	A	315	LEU	4.8
1	B	1203	ARG	4.7
1	B	1163	SER	4.7
1	B	1337	PRO	4.6
1	A	313	ASP	4.3
1	A	110	ASP	4.2
1	A	81	CYS	4.2
1	A	112	VAL	4.1
1	A	39	ALA	4.0
1	B	1034	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	3.9
1	B	1081	CYS	3.8
1	B	1312	SER	3.8
1	B	1109	THR	3.7
1	B	1234	PRO	3.7
1	A	341	LYS	3.6
1	A	340	ASN	3.6
1	B	1082	LYS	3.6
1	B	1035	ASN	3.4
1	A	38	VAL	3.4
1	A	109	THR	3.4
1	A	141	ARG	3.4
1	B	1202	ASP	3.4
1	A	142	GLU	3.3
1	A	79	VAL	3.3
1	B	1238	ASP	3.2
1	A	35	ASN	3.2
1	A	220	ASP	3.2
1	A	202	ASP	3.2
1	B	1315	LEU	3.0
1	B	1111	CYS	3.0
1	A	111	CYS	3.0
1	B	1406	ASN	3.0
1	A	22	THR	2.9
1	A	127	ILE	2.8
1	A	88	ILE	2.8
1	B	1166	ASP	2.8
1	A	251	PRO	2.8
1	A	41	CYS	2.7
1	A	70	ARG	2.7
1	A	252	SER	2.7
1	B	1141	ARG	2.6
1	A	80	ASN	2.6
1	A	203	ARG	2.5
1	B	1036	MET	2.5
1	B	1205	PHE	2.5
1	A	181	ARG	2.5
1	A	126	ASN	2.4
1	A	48	CYS	2.4
1	A	288	ARG	2.4
1	A	77	THR	2.4
1	A	267	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	2.3
1	B	1078	THR	2.3
1	B	1311	ALA	2.3
1	B	1240	HIS	2.3
1	A	182	ALA	2.3
1	A	23	LYS	2.2
1	B	1033	CYS	2.2
1	A	314	SER	2.2
1	A	148	LEU	2.1
1	A	125	LYS	2.1
1	B	1023	LYS	2.1
1	A	128	PHE	2.1
1	A	36	MET	2.1
1	A	53	LYS	2.1
1	B	1235	ASP	2.1
1	A	8	GLU	2.0
1	A	378	ILE	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, 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	B	1501	14/15	0.69	0.30	7.71	80,83,87,89	0
3	NAG	B	1601	14/15	0.84	0.26	2.68	58,64,69,69	0
2	NAG	A	502	14/15	0.67	0.30	-	79,80,84,85	0
3	NAG	B	1602	14/15	0.82	0.31	-	69,71,73,73	0
2	NDG	A	501	14/15	0.80	0.16	-	68,71,74,77	0
3	NAG	B	1502	14/15	0.53	0.33	-	90,91,94,94	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
6	M6P	B	1500	16/16	0.94	0.12	-0.15	29,35,37,43	0
6	M6P	A	500	16/16	0.94	0.10	-0.61	40,44,46,49	0
4	NAG	A	601	14/15	0.82	0.12	-	51,53,54,55	0
5	OS	B	6002	1/1	0.84	0.16	-	77,77,77,77	1
5	OS	A	6001	1/1	0.99	0.15	-	61,61,61,61	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.