



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:31 PM BST

PDB ID : 4Z61  
Title : The plant peptide hormone receptor complex  
Authors : Chai, J.; Wang, J.  
Deposited on : 2015-04-03  
Resolution : 2.75 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

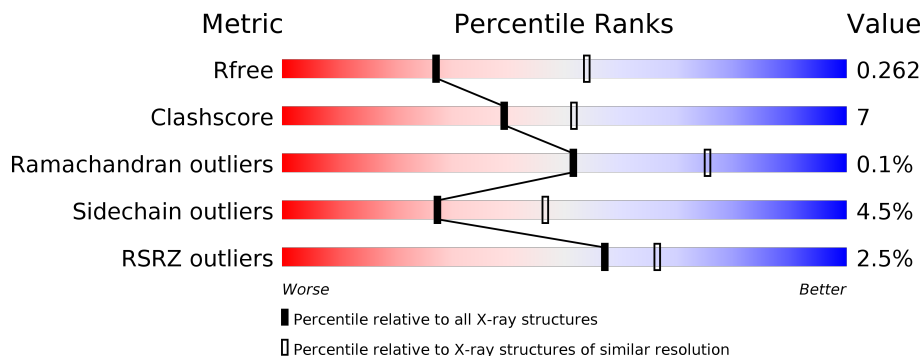
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 respectively. 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	642	
1	B	642	
2	C	222	
2	D	222	
3	P	5	
3	Q	5	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12670 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 Phytosulfokine receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	610	Total 4678	C 2964	N 789	O 907	S 18	0	0	0
1	B	603	Total 4631	C 2937	N 780	O 897	S 17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	660	HIS	-	expression tag	UNP Q8LPB4
A	661	HIS	-	expression tag	UNP Q8LPB4
A	662	HIS	-	expression tag	UNP Q8LPB4
A	663	HIS	-	expression tag	UNP Q8LPB4
A	664	HIS	-	expression tag	UNP Q8LPB4
A	665	HIS	-	expression tag	UNP Q8LPB4
B	660	HIS	-	expression tag	UNP Q8LPB4
B	661	HIS	-	expression tag	UNP Q8LPB4
B	662	HIS	-	expression tag	UNP Q8LPB4
B	663	HIS	-	expression tag	UNP Q8LPB4
B	664	HIS	-	expression tag	UNP Q8LPB4
B	665	HIS	-	expression tag	UNP Q8LPB4

- Molecule 2 is a protein called Somatic embryogenesis receptor kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	185	Total 1402	C 883	N 240	O 272	S 7	0	0	0
2	D	185	Total 1402	C 883	N 240	O 272	S 7	0	0	0

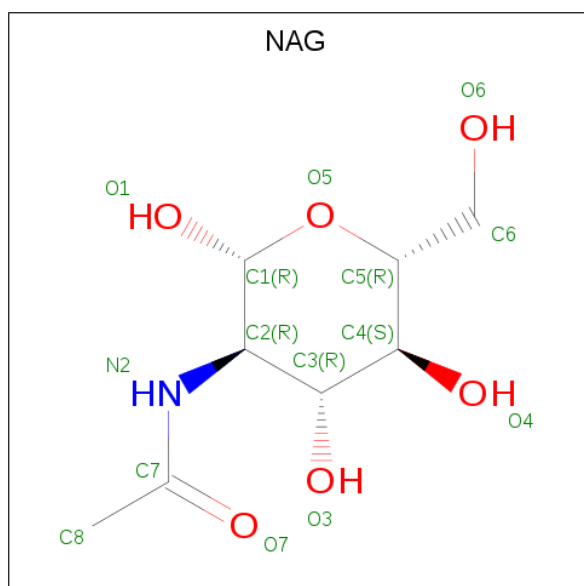
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	217	HIS	-	expression tag	UNP Q9XIC7
C	218	HIS	-	expression tag	UNP Q9XIC7
C	219	HIS	-	expression tag	UNP Q9XIC7
C	220	HIS	-	expression tag	UNP Q9XIC7
C	221	HIS	-	expression tag	UNP Q9XIC7
C	222	HIS	-	expression tag	UNP Q9XIC7
D	217	HIS	-	expression tag	UNP Q9XIC7
D	218	HIS	-	expression tag	UNP Q9XIC7
D	219	HIS	-	expression tag	UNP Q9XIC7
D	220	HIS	-	expression tag	UNP Q9XIC7
D	221	HIS	-	expression tag	UNP Q9XIC7
D	222	HIS	-	expression tag	UNP Q9XIC7

- Molecule 3 is a protein called PTR-ILE-PTR-THR-GLN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	P	5	Total	C	N	O	S	0	0	0
			57	33	6	16	2			
3	Q	5	Total	C	N	O	S	0	0	0
			57	33	6	16	2			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	0	0
			103	103		
5	B	60	Total	O	0	0
			60	60		
5	C	25	Total	O	0	0
			25	25		

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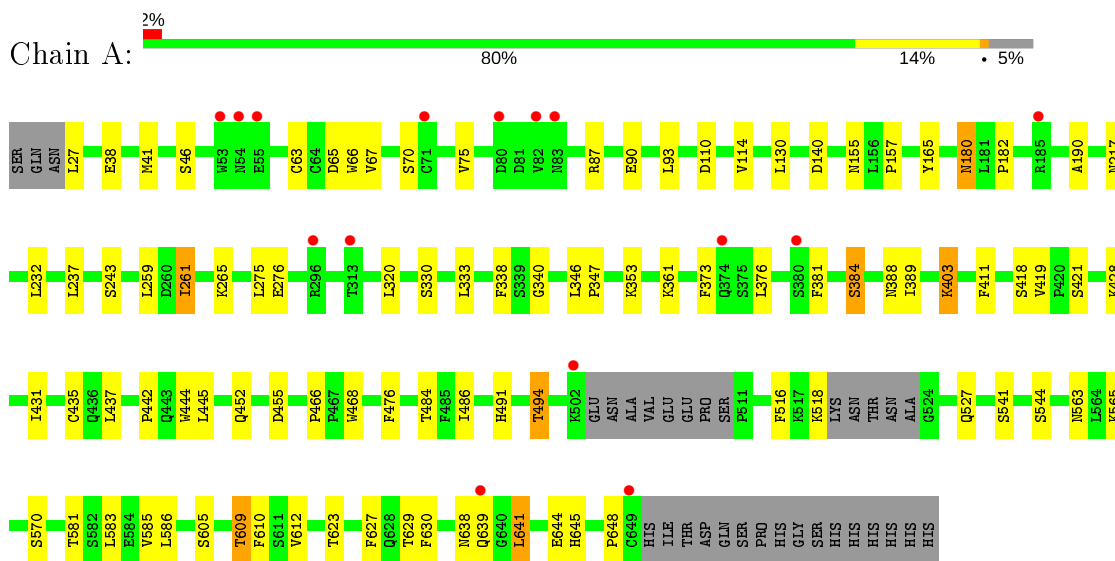
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	D	16	Total O 16 16	0	0
5	Q	1	Total O 1 1	0	0

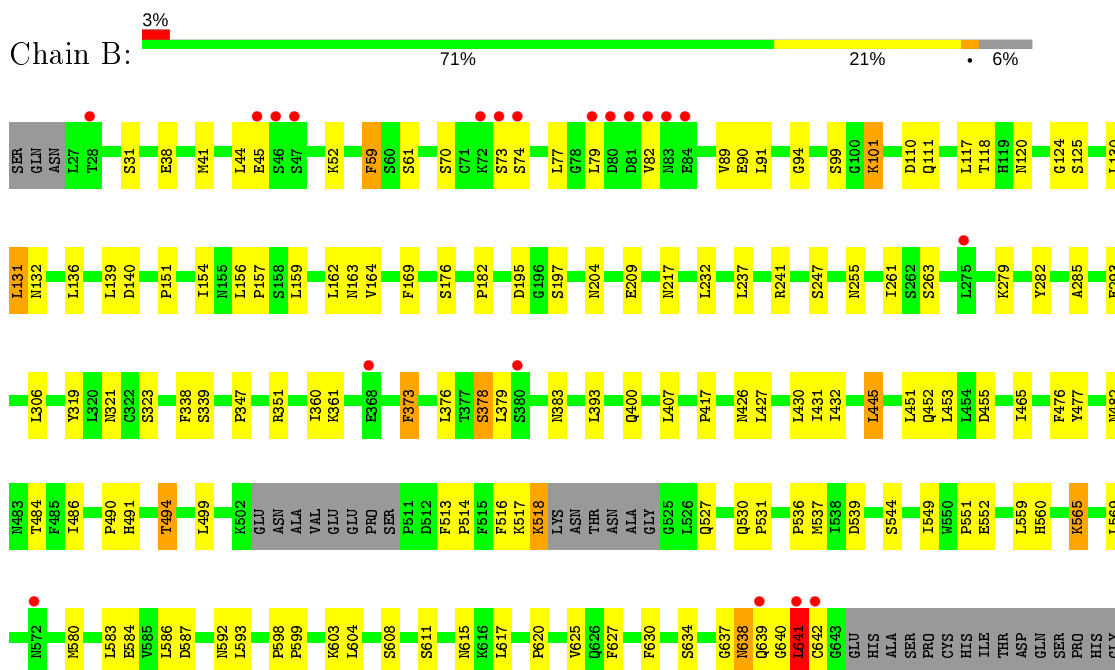
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Phytosulfokine receptor 1

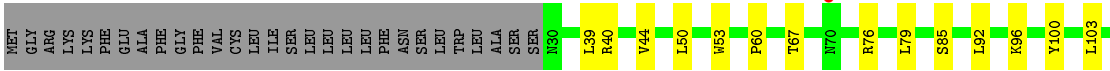


- Molecule 1: Phytosulfokine receptor 1

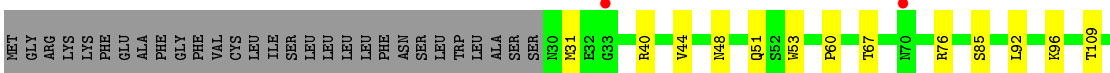


SER  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 2: Somatic embryogenesis receptor kinase 2



• Molecule 2: Somatic embryogenesis receptor kinase 2

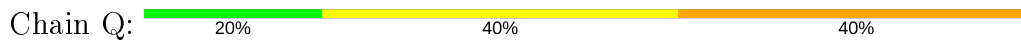


• Molecule 3: PTR-ILE-PTR-THR-GLN



Y28 I29 Y30 T31 Q32

• Molecule 3: PTR-ILE-PTR-THR-GLN



Y28 I29 Y30 T31 Q32



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	486.19Å 73.50Å 67.33Å 90.00° 95.84° 90.00°	Depositor
Resolution (Å)	29.87 – 2.75 29.87 – 2.75	Depositor EDS
% Data completeness (in resolution range)	87.7 (29.87-2.75) 87.6 (29.87-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.99 (at 2.76Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.196 , 0.262 0.199 , 0.262	Depositor DCC
$R_{free}$ test set	2770 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtrriage
Anisotropy	0.332	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: NAG, TYS

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	0.46	0/4769	0.66	0/6469
1	B	0.42	0/4720	0.64	1/6402 (0.0%)
2	C	0.42	0/1432	0.66	0/1963
2	D	0.44	0/1432	0.65	0/1963
3	P	1.40	0/23	1.17	0/27
3	Q	1.78	0/23	1.16	0/27
All	All	0.45	0/12399	0.65	1/16851 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	91	LEU	CA-CB-CG	5.45	127.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	641	LEU	Peptide

## 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	4678	0	4669	52	0
1	B	4631	0	4637	86	0
2	C	1402	0	1368	23	0
2	D	1402	0	1368	24	0
3	P	57	0	42	4	0
3	Q	57	0	42	2	0
4	A	126	0	117	2	0
4	B	84	0	78	2	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	103	0	0	5	0
5	B	60	0	0	1	0
5	C	25	0	0	1	0
5	D	16	0	0	3	0
5	Q	1	0	0	0	0
All	All	12670	0	12347	183	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 7.

All (183) 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:B:640:GLY:O	5:B:801:HOH:O	1.78	1.02
1:B:641:LEU:HD12	1:B:642:CYS:H	1.28	0.96
2:C:147:ARG:NH1	2:C:171:GLN:OE1	1.99	0.95
2:D:118:ASN:ND2	5:D:1601:HOH:O	2.01	0.93
1:B:637:GLY:C	1:B:638:ASN:HD22	1.71	0.93
1:B:637:GLY:O	1:B:638:ASN:ND2	2.03	0.92
1:B:70:SER:HB3	1:B:90:GLU:HB2	1.65	0.79
1:B:625:VAL:HG21	2:D:128:TYR:OH	1.84	0.76
1:B:641:LEU:CD1	1:B:642:CYS:H	1.99	0.75
2:C:141:GLY:HA3	2:C:163:SER:HB2	1.71	0.72
1:B:641:LEU:HD12	1:B:642:CYS:N	2.03	0.70
1:A:70:SER:HB2	1:A:90:GLU:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:LYS:O	2:C:121:ASN:ND2	2.25	0.69
1:B:255:ASN:HA	1:B:279:LYS:HZ3	1.60	0.67
1:B:159:LEU:HD21	1:B:162:LEU:HB2	1.77	0.67
1:B:482:ASN:HD21	4:B:706:NAG:C1	2.07	0.66
2:C:44:VAL:HB	2:C:85:SER:HB2	1.77	0.65
1:B:615:ASN:H	1:B:638:ASN:HD21	1.46	0.64
2:D:115:ASP:OD1	2:D:115:ASP:N	2.28	0.63
1:A:259:LEU:HD11	1:A:261:ILE:HD13	1.81	0.63
1:A:340:GLY:N	5:A:808:HOH:O	2.31	0.63
1:A:388:ASN:ND2	5:A:805:HOH:O	2.27	0.63
1:A:486:ILE:HG22	1:A:544:SER:HB2	1.81	0.62
1:A:320:LEU:HD12	1:A:346:LEU:HD21	1.81	0.62
1:A:491:HIS:O	1:A:494:THR:HB	2.00	0.62
1:A:445:LEU:HB3	1:A:468:TRP:HH2	1.64	0.61
1:B:431:ILE:HG23	1:B:455:ASP:HB3	1.82	0.61
1:B:565:LYS:HD2	1:B:587:ASP:OD2	2.00	0.61
2:D:40:ARG:NH1	2:D:53:TRP:O	2.33	0.61
1:B:237:LEU:HD12	1:B:261:ILE:HD11	1.83	0.61
2:C:40:ARG:NH1	2:C:53:TRP:O	2.33	0.60
2:D:143:LEU:HD12	2:D:146:LEU:HD22	1.83	0.60
1:B:38:GLU:HA	1:B:41:MET:HE3	1.82	0.60
1:A:541:SER:HB2	1:A:565:LYS:HG3	1.83	0.60
1:B:164:VAL:HB	1:B:169:PHE:HE2	1.67	0.60
1:B:400:GLN:O	1:B:426:ASN:ND2	2.35	0.60
1:B:617:LEU:HB2	1:B:638:ASN:OD1	2.02	0.59
1:B:217:ASN:OD1	1:B:241:ARG:NH2	2.35	0.59
1:B:74:SER:HB2	1:B:79:LEU:HD12	1.84	0.58
1:B:537:MET:HE3	1:B:539:ASP:HB2	1.85	0.58
2:D:141:GLY:HA3	2:D:163:SER:HB2	1.86	0.58
1:A:583:LEU:HD21	1:A:586:LEU:HD13	1.85	0.58
2:C:153:ASN:ND2	5:C:401:HOH:O	2.26	0.57
1:A:38:GLU:HA	1:A:41:MET:HE3	1.86	0.57
1:B:117:LEU:O	1:B:120:ASN:ND2	2.37	0.57
1:B:89:VAL:HG13	1:B:90:GLU:HG3	1.85	0.56
2:C:182:GLY:HA2	2:D:182:GLY:HA2	1.88	0.56
1:A:585:VAL:HG22	1:A:609:THR:HG23	1.87	0.55
2:D:187:ASN:ND2	5:D:1603:HOH:O	2.32	0.55
2:C:157:THR:HG22	2:C:179:ARG:HB2	1.88	0.55
1:A:140:ASP:HB2	4:A:701:NAG:H82	1.89	0.54
1:B:627:PHE:HA	1:B:630:PHE:CD2	2.42	0.53
1:B:536:PRO:HD2	1:B:560:HIS:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HG2	1:A:114:VAL:HB	1.91	0.53
1:B:625:VAL:CG2	2:D:128:TYR:OH	2.55	0.53
1:B:131:LEU:HD12	1:B:156:LEU:HD11	1.91	0.52
1:A:518:LYS:HE2	3:Q:28:TYS:O1	2.10	0.51
2:D:67:THR:HB	2:D:76:ARG:HB2	1.91	0.51
1:A:516:PHE:CE2	1:A:527:GLN:HB2	2.45	0.51
1:B:154:ILE:HG23	1:B:156:LEU:HD12	1.91	0.51
1:B:491:HIS:O	1:B:494:THR:HB	2.11	0.51
2:D:96:LYS:O	2:D:121:ASN:ND2	2.42	0.51
1:A:389:ILE:HB	1:A:411:PHE:CG	2.46	0.51
1:B:641:LEU:CG	1:B:642:CYS:N	2.73	0.51
2:D:122:LEU:O	5:D:1602:HOH:O	2.19	0.51
1:A:466:PRO:HB2	1:A:468:TRP:CD1	2.47	0.50
2:D:109:THR:HG22	2:D:131:SER:HB2	1.92	0.50
2:C:123:VAL:HA	2:C:146:LEU:HA	1.93	0.50
1:A:605:SER:OG	5:A:801:HOH:O	2.19	0.50
2:D:203:ASP:OD1	2:D:211:ARG:NH2	2.41	0.50
1:B:131:LEU:HD23	1:B:151:PRO:HG2	1.93	0.50
1:B:101:LYS:NZ	1:B:125:SER:H	2.09	0.50
1:B:620:PRO:HA	1:B:642:CYS:SG	2.51	0.50
1:B:615:ASN:H	1:B:638:ASN:ND2	2.09	0.50
1:A:87:ARG:NH2	1:A:110:ASP:OD1	2.45	0.49
1:B:486:ILE:HG22	1:B:544:SER:HB2	1.95	0.49
2:C:39:LEU:HD22	2:C:92:LEU:HD21	1.93	0.49
1:B:338:PHE:HB2	1:B:360:ILE:HG23	1.94	0.49
2:D:151:LEU:O	2:D:154:ASN:ND2	2.41	0.49
1:A:627:PHE:HA	1:A:630:PHE:CD2	2.48	0.49
2:C:160:ILE:HD12	2:C:184:VAL:HG22	1.95	0.49
1:A:243:SER:HA	1:A:265:LYS:O	2.13	0.49
2:D:44:VAL:HB	2:D:85:SER:HB2	1.95	0.49
1:B:195:ASP:HB3	1:B:217:ASN:HB3	1.95	0.49
1:B:499:LEU:HD22	1:B:559:LEU:HD12	1.95	0.49
1:A:452:GLN:HB3	1:A:476:PHE:CE1	2.48	0.48
2:D:121:ASN:HA	2:D:145:LYS:HD2	1.96	0.48
1:B:101:LYS:HD2	1:B:124:GLY:HA3	1.96	0.48
2:C:133:THR:HG22	2:C:155:SER:HB2	1.95	0.48
1:A:157:PRO:HA	1:A:182:PRO:HD2	1.96	0.48
1:A:67:VAL:HG21	1:B:59:PHE:HZ	1.78	0.48
1:A:403:LYS:HG3	1:A:428:LYS:HG2	1.96	0.48
1:A:419:VAL:HG13	1:A:421:SER:H	1.79	0.48
1:B:452:GLN:HB3	1:B:476:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLY:HA2	1:B:118:THR:O	2.14	0.47
1:B:465:ILE:O	1:B:490:PRO:HG3	2.14	0.47
1:B:513:PHE:HA	1:B:514:PRO:HD3	1.77	0.47
1:B:580:MET:O	1:B:604:LEU:HD22	2.14	0.47
2:D:181:SER:HA	2:D:203:ASP:O	2.14	0.47
2:C:119:LEU:O	2:C:143:LEU:HD22	2.14	0.47
2:D:157:THR:HG22	2:D:179:ARG:HB2	1.96	0.47
1:A:435:CYS:HB2	1:A:437:LEU:HG	1.94	0.47
2:C:181:SER:HA	2:C:203:ASP:O	2.14	0.47
3:P:30:TYS:CE1	3:P:30:TYS:O2	2.62	0.47
1:B:361:LYS:NZ	1:B:383:ASN:ND2	2.63	0.47
1:B:393:LEU:HD12	1:B:417:PRO:HG2	1.95	0.47
1:A:237:LEU:HB2	1:A:261:ILE:HD12	1.97	0.47
1:A:333:LEU:HB3	1:A:338:PHE:HE2	1.81	0.46
1:B:641:LEU:C	1:B:642:CYS:SG	2.94	0.46
1:B:641:LEU:HG	1:B:642:CYS:N	2.31	0.46
1:B:565:LYS:HD2	1:B:587:ASP:CG	2.36	0.46
1:B:73:SER:O	1:B:77:LEU:HG	2.15	0.46
1:A:563:ASN:OD1	1:A:565:LYS:HG2	2.16	0.46
1:A:237:LEU:HD12	1:A:261:ILE:HD11	1.98	0.45
1:B:157:PRO:HA	1:B:182:PRO:HD2	1.99	0.45
1:B:52:LYS:NZ	1:B:61:SER:HB2	2.32	0.45
1:B:603:LYS:HB3	1:B:603:LYS:NZ	2.31	0.45
1:A:623:THR:HG22	1:A:644:GLU:HG2	1.98	0.45
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.78	0.45
1:B:136:LEU:HD21	1:B:139:LEU:HB2	1.99	0.45
1:B:516:PHE:CE2	1:B:527:GLN:HB2	2.52	0.45
1:A:644:GLU:O	1:A:645:HIS:HB2	2.16	0.45
4:A:705:NAG:O3	5:A:802:HOH:O	2.21	0.45
1:B:453:LEU:HG	1:B:477:TYR:CD1	2.52	0.45
2:C:109:THR:HG22	2:C:131:SER:HB2	1.97	0.45
2:C:67:THR:HB	2:C:76:ARG:HB2	1.99	0.45
1:B:45:GLU:HB2	1:B:99:SER:HB2	1.99	0.44
1:A:63:CYS:HA	1:A:66:TRP:CD2	2.52	0.44
1:B:378:SER:HB2	1:B:513:PHE:CE2	2.52	0.44
1:A:428:LYS:HE3	5:A:810:HOH:O	2.16	0.44
1:B:641:LEU:CG	1:B:642:CYS:H	2.30	0.44
1:A:638:ASN:CB	1:A:641:LEU:HD22	2.48	0.44
2:D:135:PRO:HA	2:D:157:THR:O	2.17	0.44
1:A:638:ASN:HB2	1:A:641:LEU:HD22	1.99	0.43
1:B:361:LYS:HZ1	1:B:383:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ILE:HD11	1:B:593:LEU:HD11	1.99	0.43
1:B:282:TYR:CE2	1:B:306:LEU:HD13	2.53	0.43
1:B:407:LEU:HB2	1:B:432:ILE:HG12	2.00	0.43
1:B:140:ASP:HB2	4:B:701:NAG:H82	2.00	0.43
1:B:430:LEU:HD23	1:B:445:LEU:HD11	1.99	0.43
1:B:518:LYS:N	3:P:30:TYS:HE2	2.32	0.43
1:B:261:ILE:HG22	1:B:285:ALA:HA	2.00	0.43
3:P:29:ILE:HG21	3:P:29:ILE:HD13	1.78	0.43
1:B:427:LEU:O	1:B:451:LEU:HD23	2.17	0.43
1:B:569:LEU:O	1:B:592:ASN:N	2.48	0.43
1:A:165:TYR:HD1	1:A:190:ALA:HB3	1.84	0.43
1:B:376:LEU:HD21	1:B:379:LEU:HD22	2.01	0.42
1:A:610:PHE:CZ	1:A:612:VAL:HG13	2.54	0.42
1:A:381:PHE:O	1:A:384:SER:HB2	2.20	0.42
1:A:431:ILE:HG23	1:A:455:ASP:HB3	2.00	0.42
1:A:442:PRO:HB2	1:A:444:TRP:CD1	2.54	0.42
1:B:530:GLN:HB2	1:B:531:PRO:HD2	2.00	0.42
1:B:347:PRO:HA	1:B:373:PHE:CD1	2.55	0.42
1:B:560:HIS:ND1	1:B:584:GLU:OE2	2.47	0.42
1:A:629:THR:HB	2:C:100:TYR:CD2	2.54	0.42
3:Q:29:ILE:HG22	3:Q:30:TYS:N	2.33	0.42
1:B:638:ASN:HD22	1:B:638:ASN:N	2.09	0.42
2:C:79:LEU:HB2	2:C:103:LEU:HD23	2.01	0.42
1:A:445:LEU:HB3	1:A:468:TRP:CH2	2.50	0.41
1:A:346:LEU:N	1:A:347:PRO:HD2	2.35	0.41
1:B:209:GLU:O	1:B:232:LEU:HD12	2.19	0.41
1:B:611:SER:HA	1:B:634:SER:HB2	2.01	0.41
2:D:109:THR:HG22	2:D:131:SER:CB	2.49	0.41
1:B:551:PRO:HG2	1:B:552:GLU:OE1	2.19	0.41
1:A:232:LEU:HA	1:A:232:LEU:HD12	1.88	0.41
2:D:48:ASN:HB3	2:D:51:GLN:HB2	2.02	0.41
2:D:92:LEU:HD23	2:D:92:LEU:HA	1.91	0.41
2:D:194:THR:OG1	2:D:196:ILE:HG22	2.20	0.41
1:A:155:ASN:HA	1:A:180:ASN:HB3	2.03	0.41
1:B:583:LEU:HD21	1:B:586:LEU:HD13	2.02	0.41
1:B:598:PRO:HA	1:B:599:PRO:HD3	1.95	0.41
1:B:641:LEU:O	1:B:642:CYS:SG	2.77	0.41
1:A:629:THR:HB	2:C:100:TYR:CE2	2.56	0.41
1:A:353:LYS:O	1:A:376:LEU:HD12	2.21	0.41
1:B:319:TYR:OH	1:B:321:ASN:HB2	2.21	0.41
1:B:77:LEU:HD13	1:B:111:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HD12	1:A:261:ILE:HA	1.78	0.40
1:B:261:ILE:HA	1:B:261:ILE:HD12	1.89	0.40
2:C:50:LEU:HD22	2:C:53:TRP:CZ2	2.56	0.40
2:C:163:SER:O	2:C:166:ASN:HB2	2.21	0.40
1:B:518:LYS:HA	3:P:30:TYS:HE2	2.03	0.40
2:C:127:LEU:HB3	2:C:132:PHE:CE2	2.56	0.40
2:C:184:VAL:O	2:C:207:PRO:HD2	2.21	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	604/642 (94%)	580 (96%)	24 (4%)	0	100	100
1	B	597/642 (93%)	577 (97%)	20 (3%)	0	100	100
2	C	183/222 (82%)	179 (98%)	3 (2%)	1 (0%)	29	47
2	D	183/222 (82%)	179 (98%)	3 (2%)	1 (0%)	29	47
3	P	2/5 (40%)	2 (100%)	0	0	100	100
3	Q	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1571/1738 (90%)	1519 (97%)	50 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	60	PRO
2	D	60	PRO



### 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	552/581 (95%)	528 (96%)	24 (4%)	29	48
1	B	547/581 (94%)	516 (94%)	31 (6%)	20	36
2	C	164/201 (82%)	161 (98%)	3 (2%)	59	75
2	D	164/201 (82%)	159 (97%)	5 (3%)	41	61
3	P	3/3 (100%)	3 (100%)	0	100	100
3	Q	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1433/1570 (91%)	1369 (96%)	64 (4%)	27	46

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	46	SER
1	A	65	ASP
1	A	75	VAL
1	A	130	LEU
1	A	180	ASN
1	A	217	ASN
1	A	261	ILE
1	A	275	LEU
1	A	276	GLU
1	A	330	SER
1	A	361	LYS
1	A	373	PHE
1	A	384	SER
1	A	403	LYS
1	A	418	SER
1	A	484	THR
1	A	494	THR
1	A	570	SER
1	A	581	THR
1	A	609	THR
1	A	639	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	641	LEU
1	A	648	PRO
1	B	31	SER
1	B	44	LEU
1	B	59	PHE
1	B	82	VAL
1	B	101	LYS
1	B	110	ASP
1	B	130	LEU
1	B	131	LEU
1	B	132	ASN
1	B	163	ASN
1	B	176	SER
1	B	197	SER
1	B	204	ASN
1	B	247	SER
1	B	263	SER
1	B	293	GLU
1	B	323	SER
1	B	339	SER
1	B	351	ARG
1	B	373	PHE
1	B	378	SER
1	B	445	LEU
1	B	484	THR
1	B	494	THR
1	B	517	LYS
1	B	518	LYS
1	B	565	LYS
1	B	608	SER
1	B	638	ASN
1	B	639	GLN
1	B	641	LEU
2	C	163	SER
2	C	183	SER
2	C	210	SER
2	D	31	MET
2	D	115	ASP
2	D	163	SER
2	D	183	SER
2	D	192	LEU
3	Q	31	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	482	ASN
1	B	638	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TYS	P	28	3	15,16,17	1.99	3 (20%)	18,22,24	1.63	3 (16%)
3	TYS	Q	28	3	15,16,17	2.42	5 (33%)	18,22,24	1.60	3 (16%)
3	TYS	Q	30	3	15,16,17	2.96	6 (40%)	18,22,24	1.27	2 (11%)
3	TYS	P	30	3	15,16,17	1.56	3 (20%)	18,22,24	1.20	2 (11%)

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	TYS	P	28	3	-	2/10/11/13	0/1/1/1
3	TYS	Q	28	3	-	2/10/11/13	0/1/1/1
3	TYS	Q	30	3	-	3/10/11/13	0/1/1/1
3	TYS	P	30	3	-	3/10/11/13	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	30	TYS	CE1-CD1	-6.45	1.27	1.38
3	Q	30	TYS	CE2-CD2	-5.55	1.28	1.38
3	Q	28	TYS	CE1-CD1	-5.12	1.29	1.38
3	Q	30	TYS	OH-CZ	-4.67	1.35	1.42
3	P	28	TYS	CE1-CD1	-4.55	1.30	1.38
3	Q	28	TYS	CE2-CD2	-4.47	1.30	1.38
3	Q	28	TYS	OH-CZ	-4.12	1.35	1.42
3	Q	30	TYS	OH-S	-3.40	1.53	1.58
3	P	28	TYS	OH-CZ	-3.35	1.37	1.42
3	P	28	TYS	CE2-CD2	-3.26	1.32	1.38
3	P	30	TYS	CE2-CD2	-3.23	1.32	1.38
3	P	30	TYS	OH-CZ	-3.05	1.37	1.42
3	Q	30	TYS	CE1-CZ	-2.89	1.32	1.38
3	Q	28	TYS	CE1-CZ	-2.70	1.33	1.38
3	Q	30	TYS	CE2-CZ	-2.14	1.34	1.38
3	Q	28	TYS	CE2-CZ	-2.08	1.34	1.38
3	P	30	TYS	CE1-CD1	-2.08	1.35	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	28	TYS	O3-S-OH	5.21	118.37	105.83
3	P	28	TYS	OH-CZ-CE2	4.66	127.80	118.64
3	Q	30	TYS	O3-S-OH	4.11	115.73	105.83
3	P	30	TYS	O3-S-OH	3.56	114.39	105.83
3	Q	28	TYS	OH-CZ-CE2	3.23	124.98	118.64
3	P	28	TYS	OH-CZ-CE1	-3.10	112.56	118.64
3	Q	28	TYS	OH-CZ-CE1	-2.15	114.42	118.64
3	P	30	TYS	OH-CZ-CE1	2.12	122.81	118.64
3	Q	30	TYS	OH-S-O1	2.09	113.79	107.71
3	P	28	TYS	O3-S-OH	2.04	110.75	105.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	28	TYS	CE1-CZ-OH-S
3	Q	28	TYS	CE2-CZ-OH-S
3	Q	30	TYS	CZ-OH-S-O2
3	Q	30	TYS	CZ-OH-S-O3
3	P	30	TYS	CZ-OH-S-O1
3	P	30	TYS	CZ-OH-S-O3

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Mol	Chain	Res	Type	Atoms
3	P	28	TYS	CE1-CZ-OH-S
3	P	28	TYS	CE2-CZ-OH-S
3	Q	30	TYS	CZ-OH-S-O1
3	P	30	TYS	CZ-OH-S-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	28	TYS	1	0
3	Q	30	TYS	1	0
3	P	30	TYS	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

17 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	$\# Z  > 2$
4	NAG	A	706	1	14,14,15	0.58	0	17,19,21	1.18	2 (11%)
4	NAG	C	301	2	14,14,15	0.53	0	17,19,21	1.32	2 (11%)
4	NAG	A	702	1	14,14,15	0.53	0	17,19,21	0.90	0
4	NAG	A	709	1	14,14,15	0.49	0	17,19,21	1.39	2 (11%)
4	NAG	A	703	1	14,14,15	0.59	0	17,19,21	2.23	6 (35%)
4	NAG	B	703	1	14,14,15	0.44	0	17,19,21	1.86	2 (11%)
4	NAG	B	704	1	14,14,15	0.63	0	17,19,21	2.51	8 (47%)
4	NAG	A	704	1	14,14,15	0.49	0	17,19,21	1.07	2 (11%)
4	NAG	B	706	-	14,14,15	0.69	0	17,19,21	1.26	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	707	1	14,14,15	0.74	0	17,19,21	1.22	3 (17%)
4	NAG	D	1501	2	14,14,15	0.40	0	17,19,21	1.85	2 (11%)
4	NAG	B	702	1	14,14,15	0.55	0	17,19,21	1.94	6 (35%)
4	NAG	B	705	1	14,14,15	0.49	0	17,19,21	1.44	1 (5%)
4	NAG	A	705	1	14,14,15	0.60	0	17,19,21	2.02	4 (23%)
4	NAG	A	708	1	14,14,15	0.35	0	17,19,21	2.00	2 (11%)
4	NAG	B	701	1	14,14,15	0.59	0	17,19,21	1.06	2 (11%)
4	NAG	A	701	1	14,14,15	0.61	0	17,19,21	1.05	1 (5%)

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	NAG	A	706	1	-	0/6/23/26	0/1/1/1
4	NAG	C	301	2	-	0/6/23/26	0/1/1/1
4	NAG	A	702	1	-	3/6/23/26	0/1/1/1
4	NAG	A	709	1	-	4/6/23/26	0/1/1/1
4	NAG	A	703	1	-	2/6/23/26	0/1/1/1
4	NAG	B	703	1	-	3/6/23/26	0/1/1/1
4	NAG	B	704	1	-	4/6/23/26	0/1/1/1
4	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	706	-	-	2/6/23/26	0/1/1/1
4	NAG	A	707	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1501	2	-	2/6/23/26	0/1/1/1
4	NAG	B	702	1	-	3/6/23/26	0/1/1/1
4	NAG	B	705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1	-	1/6/23/26	0/1/1/1
4	NAG	A	708	1	-	2/6/23/26	0/1/1/1
4	NAG	B	701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	708	NAG	C1-O5-C5	7.08	121.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1501	NAG	C1-O5-C5	6.63	121.18	112.19
4	A	703	NAG	C1-O5-C5	6.27	120.69	112.19
4	B	704	NAG	C4-C3-C2	-5.03	103.65	111.02
4	B	705	NAG	O5-C5-C6	5.01	115.06	107.20
4	B	703	NAG	C1-O5-C5	4.99	118.95	112.19
4	A	705	NAG	C1-O5-C5	4.80	118.70	112.19
4	B	704	NAG	C1-O5-C5	4.26	117.96	112.19
4	B	703	NAG	C4-C3-C2	-4.23	104.82	111.02
4	B	704	NAG	O3-C3-C4	3.88	119.31	110.35
4	A	709	NAG	C2-N2-C7	-3.86	117.41	122.90
4	A	705	NAG	C3-C4-C5	-3.59	103.84	110.24
4	B	704	NAG	C2-N2-C7	-3.54	117.87	122.90
4	B	702	NAG	C1-C2-N2	3.51	116.48	110.49
4	B	702	NAG	C4-C3-C2	-3.48	105.92	111.02
4	C	301	NAG	O5-C5-C6	3.41	112.55	107.20
4	B	702	NAG	C2-N2-C7	3.23	127.50	122.90
4	A	703	NAG	O5-C1-C2	3.19	116.33	111.29
4	B	704	NAG	C3-C4-C5	-3.06	104.77	110.24
4	A	709	NAG	C1-O5-C5	3.00	116.26	112.19
4	A	705	NAG	C4-C3-C2	-2.96	106.68	111.02
4	A	703	NAG	O5-C5-C6	-2.92	102.63	107.20
4	A	705	NAG	O4-C4-C3	2.86	116.97	110.35
4	B	704	NAG	O5-C5-C6	-2.59	103.14	107.20
4	B	701	NAG	C1-O5-C5	2.56	115.66	112.19
4	A	708	NAG	O4-C4-C5	2.56	115.64	109.30
4	D	1501	NAG	C4-C3-C2	-2.46	107.41	111.02
4	B	706	NAG	C3-C4-C5	2.45	114.61	110.24
4	A	704	NAG	O5-C5-C6	2.43	111.02	107.20
4	B	702	NAG	C3-C4-C5	-2.39	105.97	110.24
4	B	706	NAG	O5-C1-C2	-2.37	107.55	111.29
4	A	701	NAG	O5-C1-C2	-2.35	107.58	111.29
4	B	704	NAG	O6-C6-C5	-2.34	103.27	111.29
4	B	702	NAG	C6-C5-C4	2.29	118.36	113.00
4	A	707	NAG	C2-N2-C7	-2.29	119.65	122.90
4	B	702	NAG	O4-C4-C5	2.28	114.96	109.30
4	B	701	NAG	C2-N2-C7	-2.23	119.73	122.90
4	C	301	NAG	C4-C3-C2	-2.20	107.79	111.02
4	A	703	NAG	C4-C3-C2	2.19	114.22	111.02
4	A	703	NAG	C3-C4-C5	2.18	114.13	110.24
4	A	706	NAG	C6-C5-C4	-2.13	108.02	113.00
4	A	704	NAG	C2-N2-C7	-2.10	119.91	122.90
4	A	707	NAG	O5-C5-C6	2.09	110.49	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	707	NAG	C1-O5-C5	-2.08	109.37	112.19
4	B	704	NAG	C1-C2-N2	2.07	114.02	110.49
4	A	706	NAG	C4-C3-C2	2.05	114.03	111.02
4	A	703	NAG	C1-C2-N2	-2.03	107.01	110.49
4	B	706	NAG	C2-N2-C7	2.01	125.77	122.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	NAG	C3-C2-N2-C7
4	B	703	NAG	C8-C7-N2-C2
4	B	703	NAG	O7-C7-N2-C2
4	B	702	NAG	C1-C2-N2-C7
4	B	702	NAG	C8-C7-N2-C2
4	B	702	NAG	O7-C7-N2-C2
4	B	704	NAG	C8-C7-N2-C2
4	B	704	NAG	O7-C7-N2-C2
4	A	709	NAG	O5-C5-C6-O6
4	B	704	NAG	O5-C5-C6-O6
4	A	703	NAG	C4-C5-C6-O6
4	A	703	NAG	O5-C5-C6-O6
4	A	702	NAG	C8-C7-N2-C2
4	B	706	NAG	O5-C5-C6-O6
4	A	709	NAG	C4-C5-C6-O6
4	A	702	NAG	O7-C7-N2-C2
4	A	708	NAG	O5-C5-C6-O6
4	B	704	NAG	C4-C5-C6-O6
4	D	1501	NAG	C4-C5-C6-O6
4	A	709	NAG	C8-C7-N2-C2
4	A	709	NAG	O7-C7-N2-C2
4	A	702	NAG	C4-C5-C6-O6
4	D	1501	NAG	O5-C5-C6-O6
4	A	708	NAG	C4-C5-C6-O6
4	B	706	NAG	C4-C5-C6-O6
4	A	705	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	NAG	1	0
4	A	705	NAG	1	0
4	B	701	NAG	1	0
4	A	701	NAG	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	610/642 (95%)	-0.39	15 (2%) 57 66	8, 18, 41, 97	0
1	B	603/642 (93%)	-0.18	20 (3%) 46 54	14, 29, 53, 117	0
2	C	185/222 (83%)	-0.27	2 (1%) 80 86	12, 26, 41, 51	0
2	D	185/222 (83%)	-0.22	3 (1%) 72 79	18, 29, 44, 57	0
3	P	3/5 (60%)	-0.59	0 100 100	19, 19, 19, 20	0
3	Q	3/5 (60%)	-0.70	0 100 100	10, 10, 11, 14	0
All	All	1589/1738 (91%)	-0.28	40 (2%) 57 66	8, 25, 46, 117	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	7.0
1	B	82	VAL	5.6
1	B	83	ASN	4.5
1	A	80	ASP	4.3
1	B	28	THR	4.2
1	A	54	ASN	3.8
1	B	84	GLU	3.7
1	B	275	LEU	3.3
1	B	81	ASP	3.2
1	B	642	CYS	3.1
2	D	70	ASN	3.1
1	B	80	ASP	2.9
1	A	55	GLU	2.8
1	B	641	LEU	2.7
1	A	639	GLN	2.7
1	B	45	GLU	2.7
1	A	83	ASN	2.6
2	D	168	MET	2.6
1	B	46	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	368	GLU	2.6
1	A	53	TRP	2.5
1	B	79	LEU	2.5
1	B	72	LYS	2.4
2	C	70	ASN	2.4
1	B	572	ASN	2.3
1	B	639	GLN	2.3
1	B	73	SER	2.3
1	A	374	GLN	2.2
1	B	47	SER	2.2
1	A	185	ARG	2.2
1	A	71	CYS	2.2
2	D	33	GLY	2.1
1	A	649	CYS	2.1
1	B	74	SER	2.1
1	A	296	ARG	2.1
1	A	502	LYS	2.1
1	B	380	SER	2.1
2	C	179	ARG	2.1
1	A	313	THR	2.1
1	A	380	SER	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	TYS	P	30	16/17	0.93	0.16	14,23,32,34	0
3	TYS	P	28	16/17	0.95	0.14	17,22,43,44	0
3	TYS	Q	30	16/17	0.96	0.10	9,11,22,28	0
3	TYS	Q	28	16/17	0.96	0.14	11,15,31,35	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	709	14/15	0.84	0.20	41,53,60,63	0
4	NAG	A	703	14/15	0.90	0.36	38,45,50,53	0
4	NAG	B	703	14/15	0.90	0.27	38,43,60,64	0
4	NAG	D	1501	14/15	0.90	0.37	34,40,48,49	0
4	NAG	B	706	14/15	0.91	0.16	28,36,39,41	0
4	NAG	B	702	14/15	0.91	0.13	15,31,35,40	0
4	NAG	B	704	14/15	0.92	0.18	19,25,30,40	0
4	NAG	A	702	14/15	0.93	0.20	29,44,56,57	0
4	NAG	B	705	14/15	0.93	0.16	16,24,30,34	0
4	NAG	C	301	14/15	0.94	0.12	32,34,39,40	0
4	NAG	A	708	14/15	0.94	0.16	14,16,19,19	0
4	NAG	B	701	14/15	0.94	0.16	15,23,33,36	0
4	NAG	A	704	14/15	0.95	0.20	13,20,27,30	0
4	NAG	A	705	14/15	0.95	0.14	11,16,21,27	0
4	NAG	A	706	14/15	0.96	0.23	18,23,30,34	0
4	NAG	A	707	14/15	0.96	0.17	13,19,23,26	0
4	NAG	A	701	14/15	0.97	0.16	10,20,27,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.