



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:27 pm GMT

PDB ID : 4Z5W  
Title : The plant peptide hormone receptor  
Authors : Chai, J.; Wang, J.; Han, Z.  
Deposited on : 2015-04-03  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

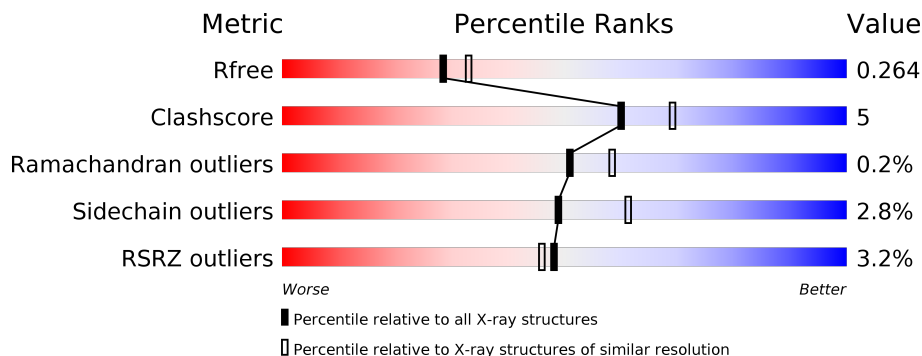
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	642	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	B	642	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>• 6%</div> </div> </div>
2	P	5	<div> <div></div> <div> <div>60%</div> <div>20%</div> <div>20%</div> </div> </div>
2	Q	5	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9842 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
1	A	596	Total	C	N	O	S	0	0	0
			4586	2910	772	888	16			
1	B	601	Total	C	N	O	S	0	0	0
			4620	2933	780	889	18			

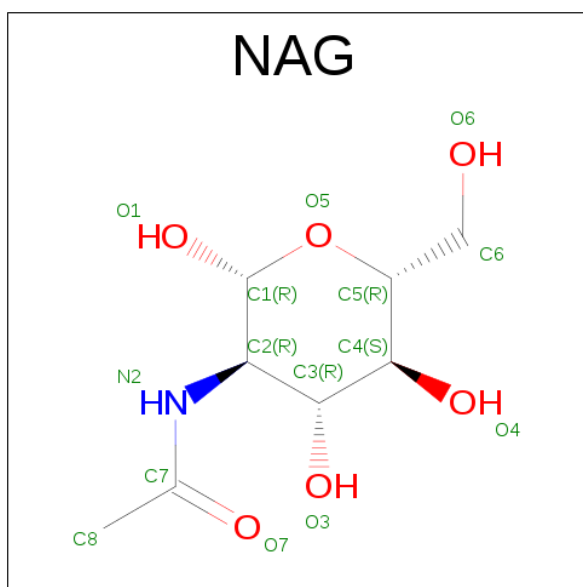
There are 12 discrepancies between the modelled and reference sequences:

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 Phytosulfokine.

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

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

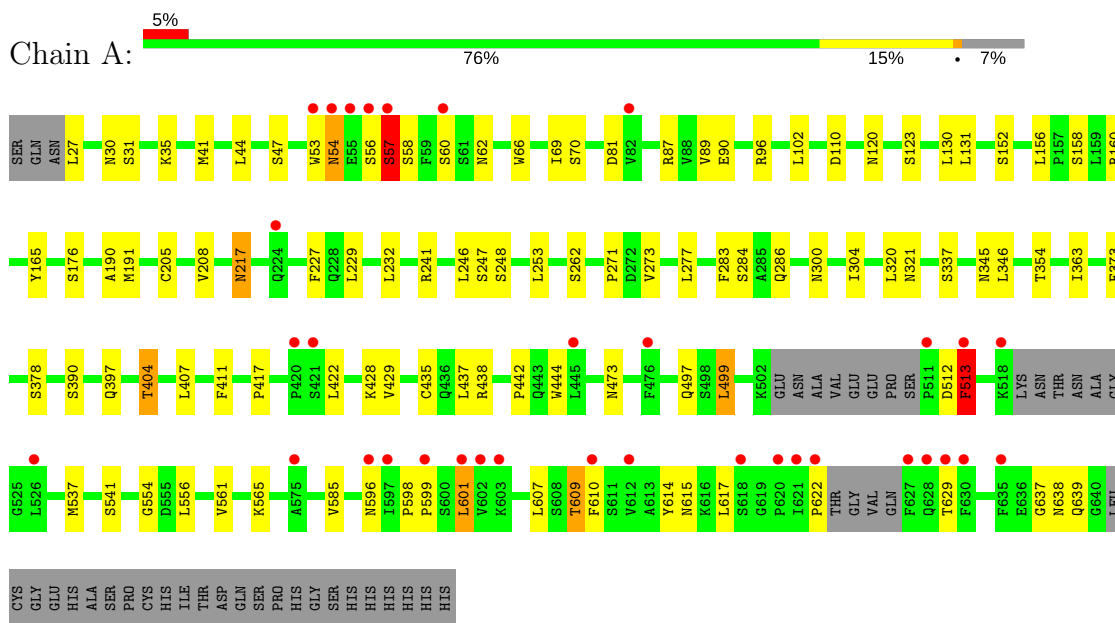
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total 119	O 119	0	0
4	B	219	Total 219	O 219	0	0
4	Q	2	Total 2	O 2	0	0

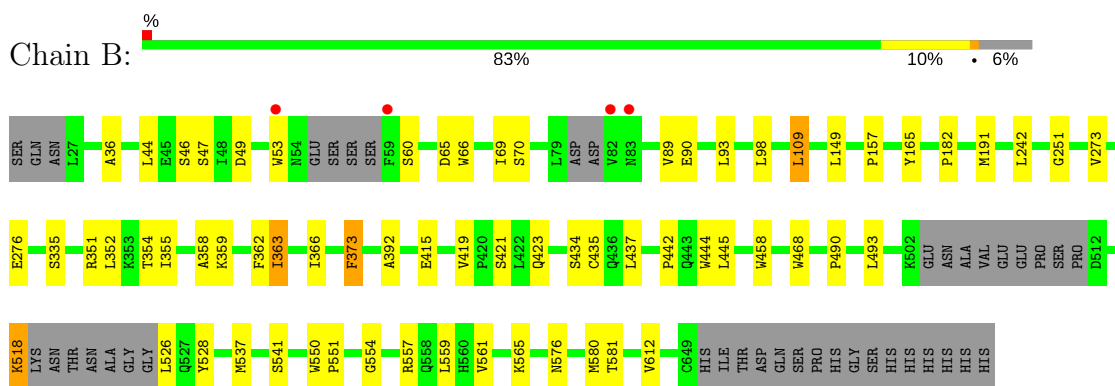
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Phytosulfokine receptor 1



#### • Molecule 1: Phytosulfokine receptor 1



#### • Molecule 2: Phytosulfokine



- Molecule 2: Phytosulfokine

Chain Q:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.67Å 75.75Å 93.90Å 111.33° 105.71° 97.17°	Depositor
Resolution (Å)	45.20 – 2.20 45.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.20-2.20) 83.9 (45.20-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.211 , 0.263 0.216 , 0.264	Depositor DCC
$R_{free}$ test set	3948 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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	0.47	1/4674 (0.0%)	0.64	0/6338
1	B	0.55	2/4708 (0.0%)	0.69	1/6384 (0.0%)
2	P	0.80	0/23	0.70	0/27
2	Q	0.41	0/23	0.61	0/27
All	All	0.51	3/9428 (0.0%)	0.67	1/12776 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	550	TRP	CB-CG	-5.86	1.39	1.50
1	B	551	PRO	N-CD	5.29	1.55	1.47
1	A	513	PHE	CD2-CE2	-5.26	1.28	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	LEU	CA-CB-CG	6.28	129.75	115.30

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	4586	0	4591	63	2
1	B	4620	0	4626	37	0
2	P	57	0	43	3	0
2	Q	57	0	44	0	0
3	A	70	0	65	2	0
3	B	112	0	103	2	0
4	A	119	0	0	4	0
4	B	219	0	0	5	0
4	Q	2	0	0	0	0
All	All	9842	0	9472	101	2

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 5.

All (101) 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:102:LEU:HD12	1:A:130:LEU:HD11	1.63	0.80
3:B:701:NAG:O6	4:B:801:HOH:O	2.08	0.69
1:A:473:ASN:ND2	1:A:497:GLN:OE1	2.27	0.68
1:B:557:ARG:NH2	4:B:809:HOH:O	2.28	0.66
1:B:490:PRO:HG2	1:B:493:LEU:HG	1.77	0.64
1:B:70:SER:HB2	1:B:90:GLU:HB2	1.80	0.64
1:A:629:THR:HB	1:B:581:THR:HG21	1.79	0.64
1:A:599:PRO:HA	1:A:622:PRO:HG3	1.82	0.62
1:A:70:SER:HB2	1:A:90:GLU:HB2	1.81	0.62
1:A:607:LEU:HD11	1:A:610:PHE:HB2	1.83	0.60
1:A:554:GLY:O	4:A:801:HOH:O	2.16	0.60
1:A:615:ASN:C	1:A:638:ASN:OD1	2.40	0.60
1:A:615:ASN:O	1:A:638:ASN:OD1	2.20	0.59
1:A:404:THR:HB	1:A:429:VAL:HB	1.85	0.58
1:B:66:TRP:HB2	1:B:69:ILE:HD12	1.85	0.58
1:A:585:VAL:HG22	1:A:609:THR:HG23	1.85	0.58
1:A:598:PRO:O	1:A:601:LEU:HD22	2.04	0.57
1:A:639:GLN:OE1	1:A:639:GLN:HA	2.04	0.57
1:A:596:ASN:OD1	4:A:802:HOH:O	2.17	0.56
1:B:541:SER:HB2	1:B:565:LYS:HG2	1.87	0.55
1:B:165:TYR:CE1	1:B:191:MET:HG3	2.42	0.55
1:A:262:SER:OG	1:A:286:GLN:HG2	2.07	0.55
1:A:87:ARG:NH2	1:A:110:ASP:OD1	2.34	0.54
1:A:165:TYR:CE1	1:A:191:MET:HG3	2.43	0.54
1:A:152:SER:O	1:A:176:SER:OG	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:O	1:A:35:LYS:HG2	2.09	0.53
1:A:321:ASN:HD21	3:A:705:NAG:C1	2.22	0.53
1:A:614:TYR:CD1	1:A:637:GLY:HA3	2.44	0.53
1:B:435:CYS:HB2	1:B:437:LEU:HG	1.91	0.52
1:A:205:CYS:O	1:A:229:LEU:HD22	2.09	0.52
1:A:513:PHE:C	1:A:513:PHE:CD1	2.83	0.52
1:B:415:GLU:OE1	4:B:803:HOH:O	2.20	0.50
1:A:54:ASN:ND2	1:A:54:ASN:N	2.60	0.49
1:A:131:LEU:HD13	1:A:156:LEU:HD11	1.95	0.48
1:A:354:THR:HG22	1:A:378:SER:HB2	1.95	0.48
1:A:30:ASN:HB2	1:A:87:ARG:HD2	1.96	0.47
1:A:617:LEU:HD12	1:A:638:ASN:ND2	2.29	0.47
1:A:47:SER:HA	1:A:53:TRP:CE2	2.49	0.47
1:A:407:LEU:HB3	1:A:411:PHE:HE2	1.78	0.47
1:B:358:ALA:HB2	2:P:31:THR:HG22	1.97	0.47
1:A:435:CYS:HB2	1:A:437:LEU:HG	1.96	0.47
1:A:397:GLN:OE1	1:A:422:LEU:HA	2.15	0.46
1:A:513:PHE:C	1:A:513:PHE:HD1	2.19	0.46
1:B:93:LEU:HB3	1:B:98:LEU:HD11	1.97	0.46
1:A:499:LEU:HB3	1:A:556:LEU:HD22	1.98	0.46
1:A:262:SER:HG	1:A:284:SER:HG	1.62	0.46
1:B:434:SER:HA	1:B:458:TRP:O	2.16	0.46
1:B:518:LYS:HD2	2:P:30:TYS:O3	2.16	0.46
1:B:554:GLY:HA2	1:B:580:MET:HG3	1.98	0.46
1:A:208:VAL:HG13	1:A:232:LEU:HD13	1.98	0.46
1:B:36:ALA:HB3	1:B:109:LEU:HD13	1.97	0.45
1:B:442:PRO:HB2	1:B:444:TRP:CD1	2.51	0.45
1:A:390:SER:HA	1:A:417:PRO:HG2	1.98	0.45
1:A:66:TRP:HB2	1:A:69:ILE:HD12	1.99	0.45
1:B:559:LEU:HD23	1:B:580:MET:CE	2.46	0.45
1:B:273:VAL:O	1:B:276:GLU:HG2	2.16	0.45
1:A:54:ASN:HD22	1:A:54:ASN:N	2.14	0.45
1:B:352:LEU:HD23	1:B:373:PHE:HZ	1.82	0.45
1:B:421:SER:O	1:B:423:GLN:HG3	2.16	0.45
1:A:320:LEU:HD13	1:A:346:LEU:HD21	1.99	0.44
1:B:157:PRO:HA	1:B:182:PRO:HD2	1.99	0.44
1:B:526:LEU:HD22	1:B:528:TYR:CE1	2.52	0.44
1:A:246:LEU:HD23	1:A:271:PRO:HD2	1.98	0.44
1:A:473:ASN:HD22	1:A:497:GLN:CD	2.19	0.44
1:A:56:SER:O	1:A:58:SER:N	2.46	0.44
1:A:614:TYR:HD1	1:A:637:GLY:HA3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:CB	2:P:31:THR:HG22	2.48	0.44
1:B:445:LEU:HB2	1:B:468:TRP:HH2	1.82	0.44
1:A:283:PHE:HB3	1:A:304:ILE:HD11	2.00	0.44
1:B:352:LEU:CD2	1:B:355:ILE:HD11	2.48	0.44
1:A:321:ASN:HD21	3:A:705:NAG:C2	2.31	0.43
1:B:251:GLY:O	1:B:276:GLU:HG3	2.18	0.43
1:B:354:THR:HG22	4:B:814:HOH:O	2.17	0.43
1:A:585:VAL:HG22	1:A:609:THR:CG2	2.48	0.43
1:B:89:VAL:HG12	1:B:90:GLU:HG3	2.01	0.43
1:A:271:PRO:HB2	1:A:273:VAL:HG13	2.00	0.42
1:A:320:LEU:O	1:A:345:ASN:ND2	2.47	0.42
1:A:512:ASP:O	1:A:513:PHE:HB2	2.19	0.42
1:B:46:SER:OG	1:B:47:SER:N	2.52	0.42
1:A:428:LYS:NZ	4:A:814:HOH:O	2.51	0.42
1:A:300:ASN:OD1	1:A:321:ASN:ND2	2.52	0.42
1:B:537:MET:HG3	1:B:561:VAL:HB	2.01	0.42
1:A:41:MET:SD	1:A:53:TRP:CD1	3.13	0.42
1:B:366:ILE:HD12	1:B:392:ALA:HB1	2.00	0.42
1:B:149:LEU:HD22	4:B:991:HOH:O	2.19	0.42
1:B:419:VAL:HG12	1:B:421:SER:H	1.84	0.42
1:A:27:LEU:O	1:A:62:ASN:ND2	2.43	0.42
1:A:541:SER:HB2	1:A:565:LYS:HG2	2.02	0.42
1:A:96:ARG:N	1:A:120:ASN:OD1	2.51	0.42
1:A:217:ASN:HD21	1:A:241:ARG:NH1	2.17	0.42
1:B:335:SER:OG	1:B:359:LYS:HE2	2.20	0.42
1:A:227:PHE:HA	1:A:253:LEU:HD21	2.02	0.41
1:A:123:SER:OG	4:A:803:HOH:O	2.20	0.41
1:A:442:PRO:HB2	1:A:444:TRP:CD1	2.56	0.41
1:B:362:PHE:C	1:B:363:ILE:HG12	2.40	0.41
1:A:165:TYR:HD1	1:A:190:ALA:HB3	1.84	0.41
1:A:89:VAL:HG12	1:A:90:GLU:HG3	2.03	0.41
1:B:363:ILE:HD12	1:B:363:ILE:HG21	1.88	0.41
3:B:701:NAG:H62	3:B:702:NAG:C7	2.51	0.40
1:A:537:MET:HG3	1:A:561:VAL:HB	2.04	0.40
1:B:352:LEU:HD21	1:B:355:ILE:HD11	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:O	1:A:248:SER:N[1_655]	1.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:O	1:A:247:SER:C[1_655]	2.14	0.06

## 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	588/642 (92%)	574 (98%)	12 (2%)	2 (0%)	44	49
1	B	591/642 (92%)	578 (98%)	13 (2%)	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
2	Q	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1183/1294 (91%)	1156 (98%)	25 (2%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	513	PHE

### 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	542/581 (93%)	524 (97%)	18 (3%)	43	54
1	B	545/581 (94%)	533 (98%)	12 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	Q	3/3 (100%)	3 (100%)	0	100	100
All	All	1093/1168 (94%)	1062 (97%)	31 (3%)	49	61

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	54	ASN
1	A	57	SER
1	A	60	SER
1	A	81	ASP
1	A	158	SER
1	A	160	ARG
1	A	217	ASN
1	A	277	LEU
1	A	337	SER
1	A	363	ILE
1	A	373	PHE
1	A	404	THR
1	A	438	ARG
1	A	499	LEU
1	A	513	PHE
1	A	601	LEU
1	A	609	THR
1	B	44	LEU
1	B	49	ASP
1	B	53	TRP
1	B	60	SER
1	B	65	ASP
1	B	242	LEU
1	B	351	ARG
1	B	363	ILE
1	B	373	PHE
1	B	518	LYS
1	B	576	ASN
1	B	612	VAL
2	P	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	A	54	ASN
1	A	217	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z  > 2$
2	TYS	P	28	2	16,16,17	2.09	4 (25%)	19,22,24	0.72	0
2	TYS	P	30	2	16,16,17	2.13	3 (18%)	19,22,24	0.52	0
2	TYS	Q	28	2	16,16,17	2.13	3 (18%)	19,22,24	0.74	1 (5%)
2	TYS	Q	30	2	16,16,17	1.97	3 (18%)	19,22,24	0.76	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
2	TYS	P	28	2	-	0/9/11/13	0/1/1/1
2	TYS	P	30	2	-	0/9/11/13	0/1/1/1
2	TYS	Q	28	2	-	0/9/11/13	0/1/1/1
2	TYS	Q	30	2	-	0/9/11/13	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	28	TYS	OH-CZ	-7.65	1.30	1.42
2	P	30	TYS	OH-CZ	-7.60	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	28	TYS	OH-CZ	-7.14	1.31	1.42
2	Q	30	TYS	OH-CZ	-6.79	1.32	1.42
2	Q	28	TYS	CA-C	2.02	1.52	1.50
2	P	28	TYS	CA-C	2.04	1.52	1.50
2	P	30	TYS	O2-S	2.18	1.53	1.45
2	P	30	TYS	O1-S	2.20	1.53	1.45
2	Q	30	TYS	O2-S	2.34	1.54	1.45
2	P	28	TYS	O2-S	2.40	1.54	1.45
2	Q	30	TYS	CA-C	2.45	1.53	1.50
2	P	28	TYS	O1-S	2.45	1.54	1.45
2	Q	28	TYS	O2-S	2.45	1.54	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	30	TYS	O-C-CA	-2.29	118.70	125.02
2	Q	28	TYS	OH-CZ-CE2	2.06	122.56	118.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	30	TYS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	701	1	14,14,15	0.61	0	15,19,21	1.57	1 (6%)
3	NAG	A	702	1	14,14,15	0.59	0	15,19,21	0.74	0
3	NAG	A	703	1	14,14,15	0.67	0	15,19,21	1.30	1 (6%)
3	NAG	A	704	1	14,14,15	0.51	0	15,19,21	0.98	0
3	NAG	A	705	-	14,14,15	0.54	0	15,19,21	1.43	3 (20%)
3	NAG	B	701	1,3	14,14,15	0.57	0	15,19,21	1.16	3 (20%)
3	NAG	B	702	3	14,14,15	0.63	0	15,19,21	0.72	1 (6%)
3	NAG	B	703	1	14,14,15	0.41	0	15,19,21	1.31	2 (13%)
3	NAG	B	704	1	14,14,15	0.67	0	15,19,21	1.14	2 (13%)
3	NAG	B	705	1	14,14,15	0.49	0	15,19,21	1.24	2 (13%)
3	NAG	B	706	1	14,14,15	0.56	0	15,19,21	1.47	2 (13%)
3	NAG	B	707	1	14,14,15	0.55	0	15,19,21	1.01	2 (13%)
3	NAG	B	708	1	14,14,15	0.67	0	15,19,21	1.34	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
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	704	1	-	0/6/23/26	0/1/1/1
3	NAG	A	705	-	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	704	1	-	0/6/23/26	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
3	NAG	B	706	1	-	0/6/23/26	0/1/1/1
3	NAG	B	707	1	-	0/6/23/26	0/1/1/1
3	NAG	B	708	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	O5-C1-C2	-4.78	104.81	111.47
3	B	708	NAG	O5-C1-C2	-4.16	105.68	111.47
3	A	705	NAG	O5-C1-C2	-3.29	106.90	111.47
3	B	704	NAG	O5-C1-C2	-2.95	107.37	111.47
3	A	705	NAG	C1-O5-C5	-2.75	108.37	112.17
3	B	706	NAG	C3-C4-C5	-2.43	105.94	110.22
3	B	701	NAG	C2-N2-C7	-2.43	119.41	122.94
3	B	704	NAG	C3-C4-C5	-2.24	106.26	110.22
3	B	701	NAG	O5-C1-C2	-2.15	108.48	111.47
3	B	705	NAG	O5-C1-C2	-2.11	108.53	111.47
3	B	703	NAG	C4-C3-C2	-2.07	107.99	111.02
3	B	702	NAG	C2-N2-C7	-2.01	120.01	122.94
3	B	707	NAG	O5-C1-C2	2.14	114.45	111.47
3	B	701	NAG	C1-O5-C5	2.38	115.44	112.17
3	A	705	NAG	C3-C4-C5	2.45	114.54	110.22
3	B	707	NAG	C1-O5-C5	2.66	115.83	112.17
3	B	705	NAG	C1-O5-C5	2.87	116.12	112.17
3	B	703	NAG	C1-O5-C5	3.01	116.31	112.17
3	B	706	NAG	C1-O5-C5	3.51	117.00	112.17
3	A	703	NAG	C1-O5-C5	3.59	117.11	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	NAG	2	0
3	B	701	NAG	2	0
3	B	702	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	596/642 (92%)	0.29	34 (5%) 24 24	7, 26, 52, 81	0
1	B	601/642 (93%)	-0.03	4 (0%) 87 86	3, 14, 38, 73	0
2	P	3/5 (60%)	-0.14	0 100 100	3, 3, 6, 7	0
2	Q	3/5 (60%)	-0.54	0 100 100	13, 13, 13, 18	0
All	All	1203/1294 (92%)	0.13	38 (3%) 48 46	3, 21, 48, 81	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	620	PRO	6.6
1	A	602	VAL	5.5
1	A	54	ASN	4.9
1	B	53	TRP	4.9
1	A	55	GLU	4.7
1	A	420	PRO	4.4
1	A	57	SER	4.4
1	A	635	PHE	4.2
1	A	596	ASN	4.1
1	A	622	PRO	4.1
1	B	59	PHE	4.0
1	A	627	PHE	3.9
1	A	601	LEU	3.7
1	A	56	SER	3.7
1	A	628	GLN	3.4
1	A	53	TRP	3.2
1	A	630	PHE	3.1
1	A	421	SER	3.1
1	A	597	ILE	3.0
1	A	612	VAL	3.0
1	A	603	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	610	PHE	2.9
1	A	60	SER	2.9
1	A	511	PRO	2.8
1	A	513	PHE	2.7
1	A	599	PRO	2.6
1	A	618	SER	2.4
1	A	224	GLN	2.4
1	A	629	THR	2.3
1	A	621	ILE	2.3
1	A	526	LEU	2.3
1	A	445	LEU	2.3
1	A	575	ALA	2.3
1	B	83	ASN	2.2
1	A	476	PHE	2.2
1	A	518	LYS	2.1
1	A	82	VAL	2.1
1	B	82	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	TYS	Q	30	16/17	0.97	0.10	-	11,15,32,33	0
2	TYS	Q	28	16/17	0.97	0.11	-	12,15,32,34	0
2	TYS	P	28	16/17	0.98	0.11	-	2,5,17,18	0
2	TYS	P	30	16/17	0.95	0.13	-	2,3,17,19	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	705	14/15	0.82	0.17	1.71	31,42,48,56	0
3	NAG	B	706	14/15	0.92	0.15	0.40	13,25,34,35	0
3	NAG	A	701	14/15	0.96	0.13	0.30	10,16,21,22	0
3	NAG	B	703	14/15	0.91	0.12	0.07	10,21,26,27	0
3	NAG	A	703	14/15	0.92	0.12	-0.13	13,20,31,40	0
3	NAG	B	705	14/15	0.95	0.12	-0.81	6,18,26,31	0
3	NAG	B	707	14/15	0.96	0.09	-1.48	18,27,36,36	0
3	NAG	A	702	14/15	0.96	0.11	-	11,22,28,33	0
3	NAG	A	704	14/15	0.88	0.17	-	27,37,42,49	0
3	NAG	B	704	14/15	0.93	0.10	-	2,11,22,24	0
3	NAG	B	708	14/15	0.88	0.12	-	11,20,25,32	0
3	NAG	B	702	14/15	0.91	0.13	-	34,44,58,63	0
3	NAG	B	701	14/15	0.97	0.13	-	2,15,25,30	0

## 6.5 Other polymers

There are no such residues in this entry.