



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:30 PM BST

PDB ID : 4Z64  
Title : the plant peptide hormone receptor complex in arabidopsis  
Authors : Chai, J.; Wang, J.; Han, Z.  
Deposited on : 2015-04-03  
Resolution : 2.66 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

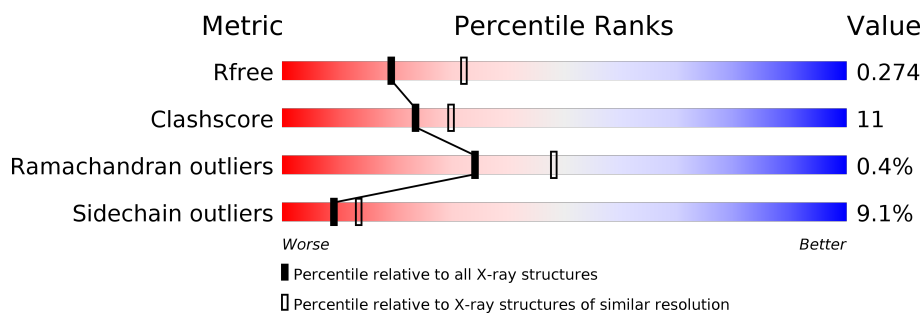
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




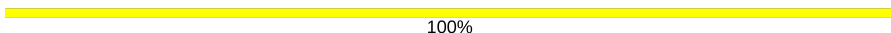
The reported resolution of this entry is 2.66 Å.

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	631	
2	C	219	
3	P	5	
4	B	2	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6364 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	605	Total	C	N	O	S	0	0	0
			4715	2986	822	888	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	649	HIS	-	expression tag	UNP Q9ZVR7
A	650	HIS	-	expression tag	UNP Q9ZVR7
A	651	HIS	-	expression tag	UNP Q9ZVR7
A	652	HIS	-	expression tag	UNP Q9ZVR7
A	653	HIS	-	expression tag	UNP Q9ZVR7
A	654	HIS	-	expression tag	UNP Q9ZVR7

- Molecule 2 is a protein called Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	186	Total	C	N	O	S	0	0	0
			1418	895	240	278	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	115	ASP	ASN	engineered mutation	UNP Q94AG2
C	163	GLN	ASN	engineered mutation	UNP Q94AG2
C	214	HIS	-	expression tag	UNP Q94AG2
C	215	HIS	-	expression tag	UNP Q94AG2
C	216	HIS	-	expression tag	UNP Q94AG2
C	217	HIS	-	expression tag	UNP Q94AG2
C	218	HIS	-	expression tag	UNP Q94AG2
C	219	HIS	-	expression tag	UNP Q94AG2

- Molecule 3 is a protein called Phytosulfokine.

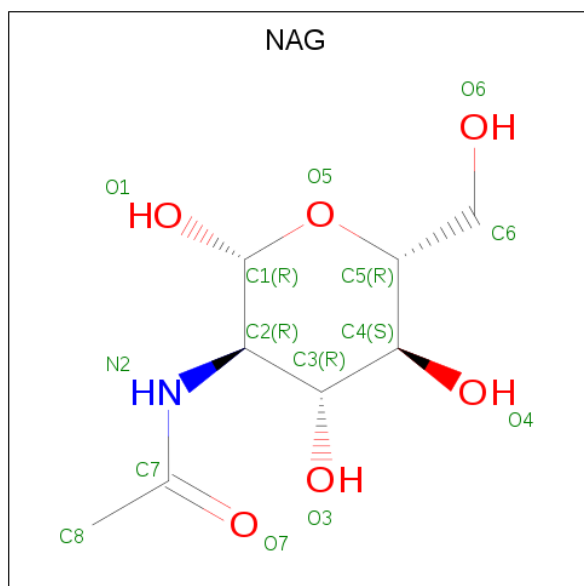
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	5	Total	C	N	O	S	0	0	0
			57	33	6	16	2			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

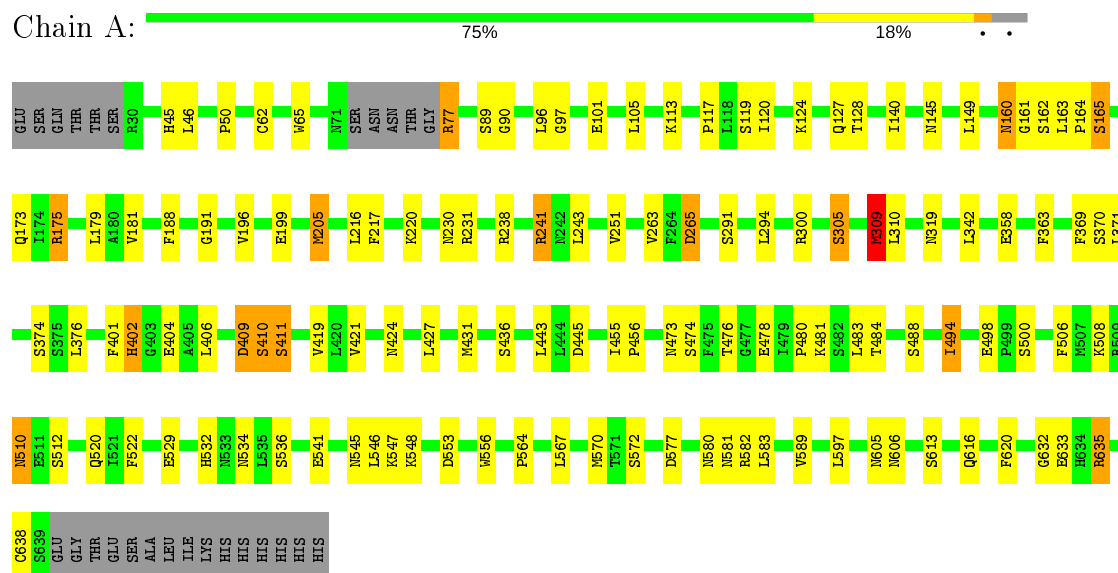


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O S	0	0
			5	4 1		
6	A	1	Total	O S	0	0
			5	4 1		
6	A	1	Total	O S	0	0
			5	4 1		
6	C	1	Total	O S	0	0
			5	4 1		

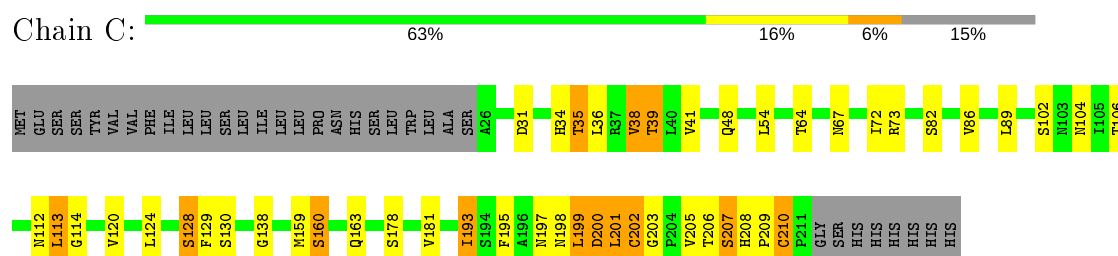
### 3 Residue-property plots

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. 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. 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.

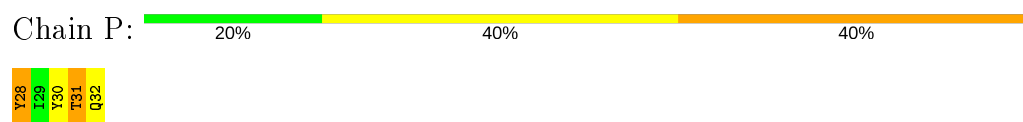
#### • Molecule 1: Phytosulfokine receptor 1



#### • Molecule 2: Somatic embryogenesis receptor kinase 1



#### • Molecule 3: Phytosulfokine



#### • Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.54Å 220.89Å 105.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.66 48.91 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.91-2.66) 95.6 (48.91-2.66)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.200 , 0.246 0.247 , 0.274	Depositor DCC
$R_{free}$ test set	2516 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: SO4, 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	0.56	0/4816	0.62	1/6524 (0.0%)
2	C	0.48	1/1448 (0.1%)	0.63	0/1986
3	P	0.42	0/23	0.73	0/27
All	All	0.54	1/6287 (0.0%)	0.62	1/8537 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	202	CYS	CB-SG	-5.21	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	MET	CG-SD-CE	-6.39	89.97	100.20

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	4715	0	4680	79	2
2	C	1418	0	1405	62	0
3	P	57	0	44	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	25	0	0
5	A	112	0	104	0	0
5	C	14	0	13	0	0
6	A	15	0	0	1	0
6	C	5	0	0	0	0
All	All	6364	0	6271	141	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 11.

All (141) 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)
2:C:208:HIS:ND1	2:C:209:PRO:HD2	1.02	1.32
2:C:208:HIS:ND1	2:C:209:PRO:CD	1.98	1.25
1:A:583:LEU:HD12	1:A:605:ASN:ND2	1.60	1.15
2:C:178:SER:OG	2:C:199:LEU:CD2	1.97	1.13
2:C:198:ASN:HD22	2:C:201:LEU:CD1	1.65	1.09
1:A:583:LEU:HB2	1:A:605:ASN:HD22	1.15	1.09
2:C:208:HIS:CE1	2:C:209:PRO:HD2	1.91	1.06
2:C:39:THR:HG21	2:C:86:VAL:CG1	1.88	1.03
2:C:198:ASN:CB	2:C:201:LEU:HD12	1.93	0.98
1:A:583:LEU:HD12	1:A:605:ASN:HD21	1.17	0.97
2:C:202:CYS:HA	2:C:206:THR:HG21	1.46	0.95
2:C:138:GLY:HA3	2:C:160:SER:HB3	1.48	0.95
2:C:198:ASN:ND2	2:C:201:LEU:CD1	2.30	0.94
1:A:583:LEU:CD1	1:A:605:ASN:HD21	1.83	0.92
2:C:181:VAL:CG2	2:C:201:LEU:HD22	2.01	0.91
1:A:300:ARG:NH1	6:A:712:SO4:O3	2.03	0.91
1:A:160:ASN:HD22	1:A:161:GLY:H	1.18	0.90
2:C:198:ASN:HB2	2:C:201:LEU:HD12	1.54	0.89
2:C:178:SER:OG	2:C:199:LEU:HD23	1.72	0.89
1:A:583:LEU:HB2	1:A:605:ASN:ND2	1.90	0.86
2:C:39:THR:HG21	2:C:86:VAL:HG11	1.56	0.86
2:C:181:VAL:HG22	2:C:201:LEU:HD22	1.56	0.86
1:A:583:LEU:CD1	1:A:605:ASN:ND2	2.38	0.86
1:A:402:HIS:H	1:A:402:HIS:CD2	1.94	0.84
1:A:160:ASN:HD22	1:A:161:GLY:N	1.74	0.83
2:C:181:VAL:HG22	2:C:201:LEU:CD2	2.08	0.83
1:A:583:LEU:CB	1:A:605:ASN:HD22	1.92	0.82
2:C:195:PHE:CD2	2:C:205:VAL:HG11	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:HIS:CG	2:C:209:PRO:HD2	2.14	0.81
1:A:251:VAL:O	1:A:251:VAL:CG1	2.30	0.80
1:A:160:ASN:ND2	1:A:161:GLY:N	2.30	0.79
2:C:198:ASN:HD22	2:C:201:LEU:HD12	1.48	0.77
2:C:205:VAL:O	2:C:205:VAL:CG1	2.33	0.77
1:A:160:ASN:ND2	1:A:161:GLY:H	1.82	0.77
2:C:198:ASN:ND2	2:C:201:LEU:HD12	1.99	0.76
1:A:583:LEU:CB	1:A:605:ASN:ND2	2.49	0.75
2:C:178:SER:OG	2:C:199:LEU:HD21	1.83	0.75
2:C:203:GLY:O	2:C:206:THR:HG22	1.86	0.75
1:A:140:ILE:HG13	1:A:164:PRO:HG3	1.67	0.74
1:A:251:VAL:O	1:A:251:VAL:HG12	1.88	0.74
2:C:205:VAL:HG12	2:C:205:VAL:O	1.89	0.72
1:A:597:LEU:O	1:A:616:GLN:HG2	1.88	0.72
1:A:488:SER:HA	1:A:494:ILE:HG21	1.72	0.71
1:A:371:LEU:HD13	1:A:376:LEU:HD11	1.73	0.71
2:C:35:THR:O	2:C:39:THR:HG22	1.90	0.71
1:A:409:ASP:OD1	1:A:409:ASP:C	2.29	0.70
1:A:406:LEU:HD13	1:A:427:LEU:HD13	1.76	0.67
1:A:409:ASP:OD1	1:A:411:SER:N	2.28	0.67
1:A:583:LEU:CG	1:A:605:ASN:ND2	2.58	0.66
2:C:206:THR:HG23	2:C:208:HIS:O	1.95	0.66
2:C:198:ASN:ND2	2:C:201:LEU:HD11	2.09	0.66
2:C:34:HIS:O	2:C:38:VAL:HG22	1.97	0.65
1:A:510:ASN:OD1	1:A:512:SER:N	2.30	0.65
2:C:181:VAL:CG2	2:C:201:LEU:CD2	2.71	0.65
1:A:583:LEU:CG	1:A:605:ASN:HD21	2.09	0.64
2:C:202:CYS:CA	2:C:206:THR:HG21	2.25	0.64
1:A:175:ARG:NH1	1:A:199:GLU:OE1	2.33	0.61
2:C:198:ASN:CG	2:C:201:LEU:HD12	2.23	0.60
2:C:178:SER:HG	2:C:199:LEU:HD21	1.66	0.59
1:A:510:ASN:OD1	1:A:510:ASN:C	2.40	0.59
1:A:498:GLU:HB2	1:A:522:PHE:CE2	2.38	0.59
2:C:178:SER:HG	2:C:199:LEU:CD2	2.11	0.59
2:C:195:PHE:HD2	2:C:205:VAL:HG11	1.68	0.58
2:C:203:GLY:N	2:C:206:THR:CG2	2.67	0.57
2:C:203:GLY:O	2:C:206:THR:CG2	2.51	0.57
2:C:198:ASN:HD22	2:C:201:LEU:HD13	1.66	0.57
2:C:39:THR:HG21	2:C:86:VAL:HG13	1.83	0.56
1:A:580:ASN:C	1:A:581:ASN:HD22	2.08	0.56
1:A:476:THR:HA	1:A:534:ASN:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:HG13	1:A:443:LEU:HD22	1.88	0.55
1:A:620:PHE:O	1:A:635:ARG:NH1	2.38	0.55
1:A:583:LEU:H	1:A:605:ASN:ND2	2.04	0.55
1:A:632:GLY:HA3	1:A:635:ARG:O	2.07	0.55
1:A:117:PRO:HD2	1:A:120:ILE:HD12	1.88	0.55
1:A:481:LYS:O	1:A:484:THR:OG1	2.24	0.54
2:C:31:ASP:O	2:C:35:THR:HG23	2.07	0.54
2:C:36:LEU:HD22	2:C:89:LEU:HD21	1.90	0.54
1:A:478:GLU:HA	1:A:536:SER:O	2.09	0.52
1:A:369:PHE:CE2	1:A:371:LEU:HD12	2.45	0.51
1:A:370:SER:OG	3:P:31:THR:HG21	2.10	0.51
1:A:127:GLN:HA	1:A:149:LEU:HA	1.93	0.50
2:C:206:THR:OG1	2:C:207:SER:N	2.44	0.50
1:A:421:VAL:HG13	1:A:445:ASP:HB3	1.93	0.49
1:A:251:VAL:O	1:A:251:VAL:HG13	2.12	0.49
2:C:112:ASN:O	2:C:114:GLY:N	2.46	0.49
1:A:532:HIS:CE1	1:A:556:TRP:CD1	3.01	0.49
2:C:203:GLY:N	2:C:206:THR:HG22	2.27	0.49
2:C:197:ASN:O	2:C:197:ASN:OD1	2.30	0.49
2:C:72:ILE:HG13	2:C:73:ARG:HG3	1.93	0.48
2:C:35:THR:O	2:C:38:VAL:HG23	2.14	0.48
2:C:112:ASN:O	2:C:113:LEU:C	2.52	0.48
1:A:77:ARG:HA	1:A:77:ARG:HD2	1.57	0.48
1:A:358:GLU:H	1:A:358:GLU:CD	2.16	0.48
1:A:431:MET:HG3	1:A:456:PRO:HD3	1.95	0.47
1:A:567:LEU:HD22	1:A:570:MET:HE1	1.96	0.47
1:A:424:ASN:ND2	3:P:28:TYS:O3	2.47	0.47
1:A:319:ASN:HA	1:A:342:LEU:HA	1.95	0.47
1:A:409:ASP:OD1	1:A:410:SER:N	2.47	0.47
1:A:455:ILE:O	1:A:480:PRO:HG3	2.14	0.47
1:A:506:PHE:CE2	3:P:32:GLN:HG2	2.50	0.46
1:A:217:PHE:HA	1:A:243:LEU:HD21	1.97	0.46
1:A:370:SER:CB	3:P:31:THR:HG21	2.45	0.46
2:C:208:HIS:CE1	2:C:209:PRO:CD	2.78	0.45
1:A:62:CYS:HA	1:A:65:TRP:CE2	2.51	0.45
2:C:193:ILE:H	2:C:193:ILE:HG13	1.51	0.45
1:A:265:ASP:OD1	1:A:265:ASP:N	2.43	0.44
2:C:39:THR:CG2	2:C:86:VAL:HG11	2.37	0.44
2:C:181:VAL:HG21	2:C:201:LEU:HD22	1.93	0.44
2:C:203:GLY:H	2:C:206:THR:CG2	2.31	0.44
2:C:41:VAL:HB	2:C:82:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:SER:OG	1:A:191:GLY:HA3	2.18	0.43
1:A:553:ASP:OD1	1:A:577:ASP:HB3	2.18	0.43
1:A:541:GLU:HG2	1:A:564:PRO:HB3	1.99	0.43
1:A:77:ARG:HG3	1:A:101:GLU:HG3	1.99	0.43
1:A:581:ASN:HD22	1:A:581:ASN:N	2.16	0.43
1:A:62:CYS:HA	1:A:65:TRP:CD2	2.54	0.43
1:A:181:VAL:HG22	1:A:205:MET:CG	2.49	0.43
1:A:401:PHE:O	1:A:404:GLU:HG3	2.19	0.43
1:A:370:SER:HB2	3:P:31:THR:HG21	2.01	0.42
2:C:195:PHE:HD2	2:C:205:VAL:CG1	2.30	0.42
2:C:202:CYS:SG	2:C:210:CYS:HA	2.59	0.42
2:C:64:THR:HB	2:C:73:ARG:HB2	2.00	0.42
1:A:241:ARG:HB3	1:A:263:VAL:HB	2.01	0.42
1:A:45:HIS:O	1:A:90:GLY:HA3	2.20	0.42
1:A:545:ASN:O	1:A:547:LYS:N	2.53	0.41
2:C:195:PHE:CD2	2:C:205:VAL:CG1	2.97	0.41
2:C:124:LEU:HB3	2:C:129:PHE:CE2	2.55	0.41
1:A:124:LYS:HE2	1:A:145:ASN:ND2	2.35	0.41
2:C:106:THR:HG22	2:C:128:SER:HB2	2.02	0.41
1:A:46:LEU:HA	1:A:89:SER:O	2.21	0.41
1:A:498:GLU:HB2	1:A:522:PHE:CZ	2.56	0.41
2:C:199:LEU:HD23	2:C:200:ASP:N	2.36	0.41
2:C:205:VAL:O	2:C:205:VAL:HG13	2.17	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.90	0.41
1:A:97:GLY:HA3	1:A:119:SER:HB2	2.03	0.41
1:A:230:ASN:HB3	1:A:231:ARG:H	1.73	0.41
1:A:605:ASN:HB3	1:A:606:ASN:H	1.78	0.41
1:A:163:LEU:HA	1:A:164:PRO:HD3	1.89	0.40
1:A:473:ASN:HB3	1:A:474:SER:H	1.77	0.40
1:A:581:ASN:HB3	1:A:582:ARG:H	1.75	0.40
2:C:197:ASN:O	2:C:197:ASN:CG	2.60	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:305:SER:OG	1:A:305:SER:OG[4_555]	1.64	0.56
1:A:309:MET:CG	1:A:309:MET:SD[4_555]	1.83	0.37

## 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	601/631 (95%)	546 (91%)	53 (9%)	2 (0%)	41	56
2	C	184/219 (84%)	169 (92%)	14 (8%)	1 (0%)	29	43
3	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	787/855 (92%)	717 (91%)	67 (8%)	3 (0%)	34	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	A	546	LEU
2	C	113	LEU

### 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	544/567 (96%)	500 (92%)	44 (8%)	11	17
2	C	170/201 (85%)	150 (88%)	20 (12%)	5	7
3	P	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	717/771 (93%)	652 (91%)	65 (9%)	9	13

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	96	LEU
1	A	105	LEU
1	A	113	LYS
1	A	128	THR
1	A	160	ASN
1	A	162	SER
1	A	165	SER
1	A	173	GLN
1	A	175	ARG
1	A	179	LEU
1	A	188	PHE
1	A	196	VAL
1	A	205	MET
1	A	216	LEU
1	A	220	LYS
1	A	238	ARG
1	A	241	ARG
1	A	265	ASP
1	A	291	SER
1	A	294	LEU
1	A	305	SER
1	A	309	MET
1	A	310	LEU
1	A	363	PHE
1	A	374	SER
1	A	402	HIS
1	A	409	ASP
1	A	410	SER
1	A	411	SER
1	A	436	SER
1	A	494	ILE
1	A	500	SER
1	A	508	LYS
1	A	510	ASN
1	A	520	GLN
1	A	529	GLU
1	A	548	LYS
1	A	572	SER
1	A	589	VAL
1	A	613	SER
1	A	633	GLU
1	A	635	ARG

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Mol	Chain	Res	Type
1	A	638	CYS
2	C	35	THR
2	C	38	VAL
2	C	39	THR
2	C	48	GLN
2	C	54	LEU
2	C	67	ASN
2	C	102	SER
2	C	104	ASN
2	C	120	VAL
2	C	128	SER
2	C	130	SER
2	C	159	MET
2	C	160	SER
2	C	163	GLN
2	C	193	ILE
2	C	199	LEU
2	C	200	ASP
2	C	201	LEU
2	C	207	SER
2	C	210	CYS
3	P	31	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	402	HIS
1	A	424	ASN
1	A	493	ASN
1	A	532	HIS
1	A	605	ASN
2	C	198	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

2 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	1.96	3 (20%)	18,22,24	0.62	0
3	TYS	P	30	3	15,16,17	2.03	3 (20%)	18,22,24	0.69	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
3	TYS	P	28	3	-	0/10/11/13	0/1/1/1
3	TYS	P	30	3	-	0/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	30	TYS	OH-CZ	-6.91	1.31	1.42
3	P	28	TYS	OH-CZ	-6.74	1.31	1.42
3	P	30	TYS	O1-S	2.29	1.55	1.45
3	P	28	TYS	O2-S	2.24	1.54	1.45
3	P	28	TYS	OH-S	2.23	1.61	1.58
3	P	30	TYS	O2-S	2.06	1.54	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	30	TYS	CB-CA-C	-2.38	107.01	111.47

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
3	P	28	TYS	1	0

## 5.5 Carbohydrates

2 monosaccharides 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	B	1	1,4	14,14,15	0.56	0	17,19,21	0.99	1 (5%)
4	NAG	B	2	4	14,14,15	0.53	0	17,19,21	0.88	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	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C1-O5-C5	2.51	115.59	112.19
4	B	2	NAG	O5-C5-C6	2.05	110.41	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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
6	SO4	C	1502	-	4,4,4	0.15	0	6,6,6	0.26	0
5	NAG	A	707	1	14,14,15	0.50	0	17,19,21	1.28	4 (23%)
6	SO4	A	712	-	4,4,4	0.15	0	6,6,6	0.23	0
5	NAG	A	710	1	14,14,15	0.46	0	17,19,21	1.32	1 (5%)
5	NAG	C	1501	2	14,14,15	0.43	0	17,19,21	1.43	2 (11%)
5	NAG	A	702	1	14,14,15	0.52	0	17,19,21	1.15	0
5	NAG	A	709	1	14,14,15	0.47	0	17,19,21	1.69	3 (17%)
6	SO4	A	713	-	4,4,4	0.16	0	6,6,6	0.07	0
5	NAG	A	705	1	14,14,15	0.65	0	17,19,21	2.14	7 (41%)
5	NAG	A	701	1	14,14,15	0.54	0	17,19,21	1.08	2 (11%)
5	NAG	A	706	1	14,14,15	0.60	0	17,19,21	0.92	0
5	NAG	A	708	1	14,14,15	0.50	0	17,19,21	1.20	1 (5%)
6	SO4	A	711	-	4,4,4	0.17	0	6,6,6	0.14	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
5	NAG	A	707	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	710	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1501	2	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	4/6/23/26	0/1/1/1
5	NAG	A	709	1	-	0/6/23/26	0/1/1/1
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
5	NAG	A	708	1	-	2/6/23/26	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(°)
5	A	705	NAG	C1-O5-C5	4.39	118.14	112.19
5	A	709	NAG	C2-N2-C7	4.26	128.96	122.90
5	A	709	NAG	C1-O5-C5	4.06	117.69	112.19
5	A	708	NAG	C1-O5-C5	4.05	117.68	112.19
5	A	710	NAG	C1-O5-C5	4.02	117.63	112.19
5	A	705	NAG	O4-C4-C3	3.98	119.56	110.35
5	C	1501	NAG	C1-O5-C5	3.91	117.50	112.19
5	C	1501	NAG	O5-C5-C6	3.25	112.29	107.20
5	A	705	NAG	C4-C3-C2	-2.92	106.73	111.02
5	A	707	NAG	C2-N2-C7	-2.75	118.99	122.90
5	A	705	NAG	C3-C4-C5	-2.56	105.67	110.24
5	A	705	NAG	O3-C3-C4	2.49	116.11	110.35
5	A	707	NAG	C1-O5-C5	2.37	115.40	112.19
5	A	707	NAG	O5-C5-C6	2.33	110.86	107.20
5	A	705	NAG	O7-C7-C8	-2.23	117.92	122.06
5	A	701	NAG	O5-C5-C6	2.19	110.64	107.20
5	A	709	NAG	O7-C7-N2	2.17	125.94	121.95
5	A	701	NAG	C3-C4-C5	-2.12	106.45	110.24
5	A	705	NAG	O7-C7-N2	2.11	125.82	121.95
5	A	707	NAG	C4-C3-C2	-2.02	108.05	111.02

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	710	NAG	C8-C7-N2-C2
5	A	702	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	A	710	NAG	C4-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	A	707	NAG	C4-C5-C6-O6
5	A	710	NAG	O7-C7-N2-C2
5	A	702	NAG	O7-C7-N2-C2
5	A	702	NAG	O5-C5-C6-O6
5	A	710	NAG	O5-C5-C6-O6
5	A	701	NAG	O5-C5-C6-O6
5	C	1501	NAG	C4-C5-C6-O6
5	A	707	NAG	O5-C5-C6-O6
5	A	707	NAG	C8-C7-N2-C2
5	A	708	NAG	C8-C7-N2-C2
5	C	1501	NAG	O5-C5-C6-O6
5	A	708	NAG	O7-C7-N2-C2
5	A	705	NAG	C4-C5-C6-O6
5	A	707	NAG	O7-C7-N2-C2
5	A	705	NAG	O5-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	712	SO4	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.