



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2016 – 11:18 AM GMT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

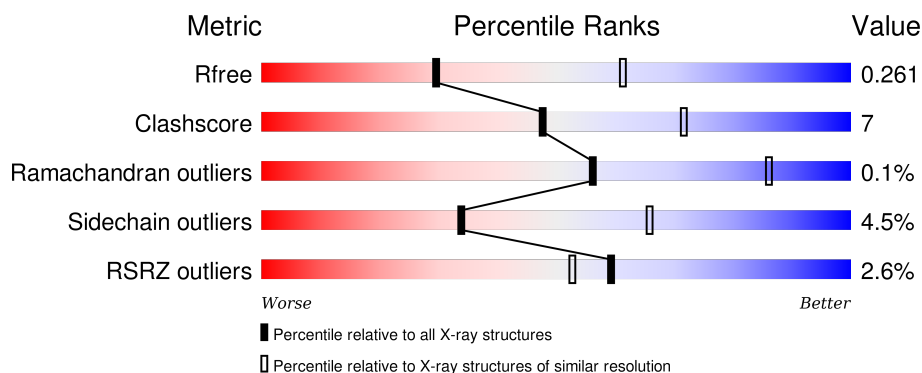
1 Overall quality at a glance

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.



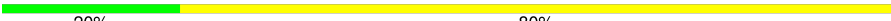
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 ≥ 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>2%</div> <div>80%</div> <div>14%</div> <div>5%</div> </div>
1	B	642	<div> <div>3%</div> <div>71%</div> <div>21%</div> <div>6%</div> </div>
2	C	222	<div> <div>%</div> <div>65%</div> <div>18%</div> <div>17%</div> </div>
2	D	222	<div> <div>%</div> <div>66%</div> <div>16%</div> <div>17%</div> </div>
3	P	5	<div> <div>60%</div> <div>40%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	702	-	-	-	X

2 Entry composition

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
1	A	610	Total	C	N	O	S	0	0	0
			4678	2964	789	907	18			
1	B	603	Total	C	N	O	S	0	0	0
			4631	2937	780	897	17			

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
2	C	185	Total	C	N	O	S	0	0	0
			1402	883	240	272	7			
2	D	185	Total	C	N	O	S	0	0	0
			1402	883	240	272	7			

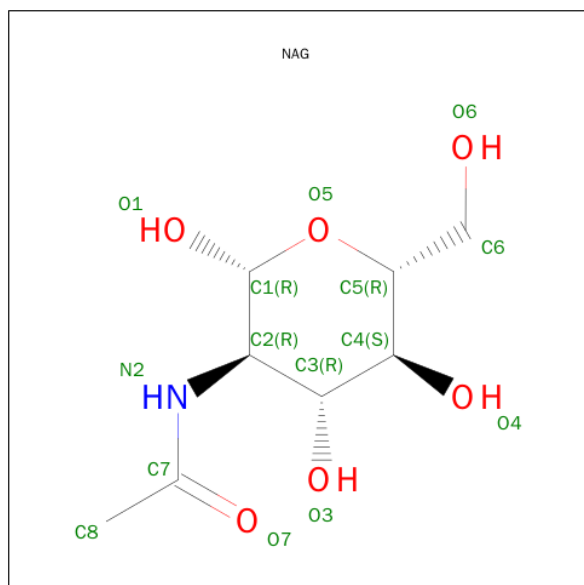
There are 12 discrepancies between the modelled and reference sequences:

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
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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		

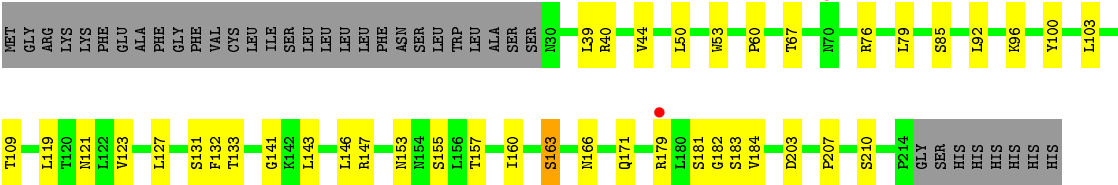
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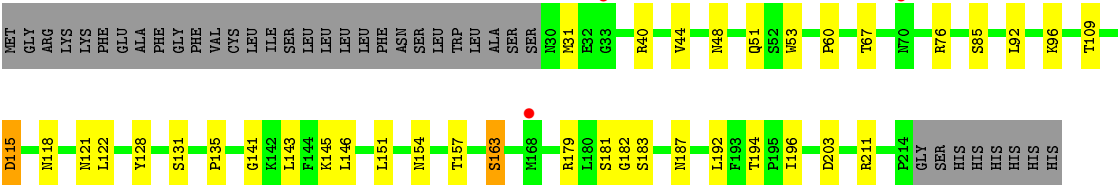
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	16	Total 16	O 16	0	0
5	Q	1	Total 1	O 1	0	0

SER
HIS
HIS
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HIS

• Molecule 2: Somatic embryogenesis receptor kinase 2



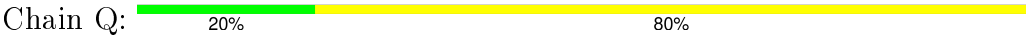
• Molecule 2: Somatic embryogenesis receptor kinase 2



• Molecule 3: PTR-ILE-PTR-THR-GLN



• Molecule 3: PTR-ILE-PTR-THR-GLN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.196 , 0.262 0.197 , 0.261	Depositor DCC
R_{free} test set	2769 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
Estimated twinning fraction	0.028 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54320 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12670	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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 ⓘ

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	34	67
2	D	183/222 (82%)	179 (98%)	3 (2%)	1 (0%)	34	67
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%)	56	86

All (2) Ramachandran outliers are listed below:

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

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	552/581 (95%)	528 (96%)	24 (4%)	35	68
1	B	547/581 (94%)	516 (94%)	31 (6%)	25	55
2	C	164/201 (82%)	161 (98%)	3 (2%)	66	90
2	D	164/201 (82%)	159 (97%)	5 (3%)	48	80
3	P	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1433/1570 (91%)	1369 (96%)	64 (4%)	34	66

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	101	LYS
1	B	197	SER
2	D	115	ASP
1	B	110	ASP
1	B	132	ASN

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 ⓘ

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$
3	TYS	P	28	3	14,16,17	2.20	4 (28%)	16,22,24	1.62	3 (18%)
3	TYS	P	30	3	14,16,17	1.90	3 (21%)	16,22,24	0.99	2 (12%)
3	TYS	Q	28	3	14,16,17	2.59	6 (42%)	16,22,24	1.16	2 (12%)
3	TYS	Q	30	3	14,16,17	3.19	6 (42%)	16,22,24	0.77	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
3	TYS	P	28	3	-	0/9/11/13	0/1/1/1
3	TYS	P	30	3	-	0/9/11/13	0/1/1/1
3	TYS	Q	28	3	-	0/9/11/13	0/1/1/1
3	TYS	Q	30	3	-	0/9/11/13	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	30	TYS	CE1-CD1	-5.94	1.27	1.38
3	Q	30	TYS	OH-S	-5.71	1.53	1.63
3	Q	30	TYS	CE2-CD2	-5.12	1.28	1.38
3	Q	30	TYS	OH-CZ	-4.85	1.35	1.42
3	Q	28	TYS	CE1-CD1	-4.72	1.29	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	28	TYS	OH-CZ-CE1	-3.20	112.56	118.77
3	P	30	TYS	O-C-CA	-2.43	119.22	125.72
3	Q	28	TYS	OH-CZ-CE1	-2.24	114.42	118.77
3	P	28	TYS	O-C-CA	-2.07	120.16	125.72
3	P	30	TYS	OH-CZ-CE1	2.09	122.81	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	701	1	14,14,15	0.59	0	15,19,21	0.94	1 (6%)
4	NAG	A	702	1	14,14,15	0.51	0	15,19,21	0.83	0
4	NAG	A	703	1	14,14,15	0.57	0	15,19,21	2.08	4 (26%)
4	NAG	A	704	1	14,14,15	0.47	0	15,19,21	1.08	1 (6%)
4	NAG	A	705	1	14,14,15	0.58	0	15,19,21	2.09	4 (26%)
4	NAG	A	706	1	14,14,15	0.56	0	15,19,21	1.11	0
4	NAG	A	707	1	14,14,15	0.71	0	15,19,21	1.25	1 (6%)
4	NAG	A	708	1	14,14,15	0.33	0	15,19,21	1.97	2 (13%)
4	NAG	A	709	1	14,14,15	0.46	0	15,19,21	1.55	2 (13%)
4	NAG	B	701	1	14,14,15	0.58	0	15,19,21	1.11	2 (13%)
4	NAG	B	702	1	14,14,15	0.53	0	15,19,21	1.82	5 (33%)
4	NAG	B	703	1	14,14,15	0.42	0	15,19,21	1.99	3 (20%)
4	NAG	B	704	1	14,14,15	0.60	0	15,19,21	2.64	7 (46%)
4	NAG	B	705	1	14,14,15	0.47	0	15,19,21	1.22	1 (6%)
4	NAG	B	706	-	14,14,15	0.67	0	15,19,21	1.22	2 (13%)
4	NAG	C	301	2	14,14,15	0.51	0	15,19,21	1.25	2 (13%)
4	NAG	D	1501	2	14,14,15	0.38	0	15,19,21	1.89	2 (13%)

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	701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	702	1	-	0/6/23/26	0/1/1/1
4	NAG	A	703	1	-	0/6/23/26	0/1/1/1
4	NAG	A	704	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	706	1	-	0/6/23/26	0/1/1/1
4	NAG	A	707	1	-	0/6/23/26	0/1/1/1
4	NAG	A	708	1	-	0/6/23/26	0/1/1/1
4	NAG	A	709	1	-	0/6/23/26	0/1/1/1
4	NAG	B	701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	703	1	-	0/6/23/26	0/1/1/1
4	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	705	1	-	0/6/23/26	0/1/1/1
4	NAG	B	706	-	-	0/6/23/26	0/1/1/1
4	NAG	C	301	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1501	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	NAG	C4-C3-C2	-4.95	103.65	111.34
4	A	709	NAG	C2-N2-C7	-4.38	117.41	123.11
4	B	703	NAG	C4-C3-C2	-4.20	104.82	111.34
4	B	704	NAG	C2-N2-C7	-4.03	117.87	123.11
4	A	705	NAG	C3-C4-C5	-3.58	103.84	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	702	NAG	O7-C7-N2-C2
4	B	702	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	NAG	1	0
4	A	705	NAG	1	0
4	B	701	NAG	1	0
4	B	706	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, 95th 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 ²)	Q<0.9
1	A	610/642 (95%)	-0.39	16 (2%) 59 53	8, 18, 41, 97	0
1	B	603/642 (93%)	-0.18	20 (3%) 50 43	14, 29, 53, 117	0
2	C	185/222 (83%)	-0.27	2 (1%) 82 78	12, 26, 41, 51	0
2	D	185/222 (83%)	-0.22	3 (1%) 74 70	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%)	-0.69	0 100 100	10, 10, 11, 14	0
All	All	1589/1738 (91%)	-0.28	41 (2%) 59 53	8, 25, 46, 117	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	7.0
1	B	82	VAL	5.5
1	B	83	ASN	4.5
1	A	80	ASP	4.2
1	B	28	THR	4.1

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

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, 95th 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 ²)	Q<0.9
3	TYS	P	28	16/17	0.95	0.14	-	17,22,43,44	0
3	TYS	Q	28	16/17	0.96	0.14	-	11,15,31,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TYS	Q	30	16/17	0.96	0.10	-	9,11,22,28	0
3	TYS	P	30	16/17	0.93	0.16	-	14,23,32,34	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, 95th 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(\AA^2)	Q<0.9
4	NAG	A	702	14/15	0.93	0.20	2.20	29,44,56,57	0
4	NAG	A	706	14/15	0.96	0.23	1.73	18,23,30,34	0
4	NAG	A	704	14/15	0.95	0.20	1.55	13,20,27,30	0
4	NAG	B	703	14/15	0.90	0.27	1.24	38,43,60,64	0
4	NAG	B	704	14/15	0.92	0.18	1.08	19,25,30,40	0
4	NAG	A	709	14/15	0.84	0.20	0.85	41,53,60,63	0
4	NAG	A	701	14/15	0.97	0.16	0.47	10,20,27,29	0
4	NAG	B	701	14/15	0.94	0.16	0.04	15,23,33,36	0
4	NAG	C	301	14/15	0.94	0.12	-0.02	32,34,39,40	0
4	NAG	A	708	14/15	0.94	0.16	-0.12	14,16,19,19	0
4	NAG	A	707	14/15	0.96	0.17	-0.22	13,19,23,26	0
4	NAG	A	705	14/15	0.96	0.14	-0.28	11,16,21,27	0
4	NAG	B	702	14/15	0.91	0.13	-0.33	15,31,35,40	0
4	NAG	A	703	14/15	0.90	0.35	-	38,45,50,53	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	705	14/15	0.93	0.16	-	16,24,30,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.