Full wwPDB X-ray Structure Validation Report (i)

Sep 21, 2016 – 08:07 AM EDT

PDB ID	:	5IYX
Title	:	Crystal structure of the Arabidopsis receptor kinase HAESA in complex with the peptide hormone IDA and the co-receptor SERK1
Authors	:	Santiago, J.; Hothorn, M.
Deposited on	:	2016-03-24
Resolution	:	2.43 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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

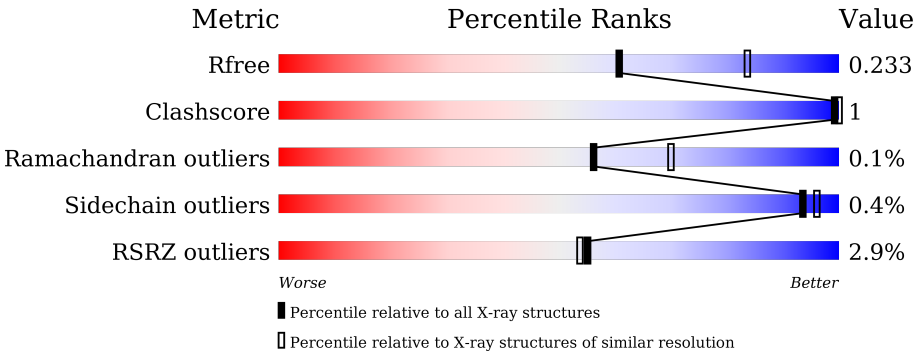
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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 <=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	658	3%, 88%, 9%
2	B	14	93%, 7%
3	C	201	91%, 7%

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
5	EDO	A	712	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6388 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 Receptor-like protein kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4543	2878	768	883	14	0	1	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP P47735
A	16	SER	-	expression tag	UNP P47735
A	17	SER	-	expression tag	UNP P47735
A	18	MET	-	expression tag	UNP P47735
A	19	GLY	-	expression tag	UNP P47735
A	621	LEU	-	expression tag	UNP P47735
A	622	GLU	-	expression tag	UNP P47735
A	623	GLY	-	expression tag	UNP P47735
A	624	SER	-	expression tag	UNP P47735
A	625	GLU	-	expression tag	UNP P47735
A	626	ASN	-	expression tag	UNP P47735
A	627	LEU	-	expression tag	UNP P47735
A	628	TYR	-	expression tag	UNP P47735
A	629	PHE	-	expression tag	UNP P47735
A	630	GLN	-	expression tag	UNP P47735
A	631	GLY	-	expression tag	UNP P47735
A	632	SER	-	expression tag	UNP P47735
A	633	ALA	-	expression tag	UNP P47735
A	634	TRP	-	expression tag	UNP P47735
A	635	SER	-	expression tag	UNP P47735
A	636	HIS	-	expression tag	UNP P47735
A	637	PRO	-	expression tag	UNP P47735
A	638	GLN	-	expression tag	UNP P47735
A	639	PHE	-	expression tag	UNP P47735
A	640	GLU	-	expression tag	UNP P47735
A	641	LYS	-	expression tag	UNP P47735
A	642	GLY	-	expression tag	UNP P47735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	643	GLY	-	expression tag	UNP P47735
A	644	GLY	-	expression tag	UNP P47735
A	645	SER	-	expression tag	UNP P47735
A	646	GLY	-	expression tag	UNP P47735
A	647	GLY	-	expression tag	UNP P47735
A	648	GLY	-	expression tag	UNP P47735
A	649	SER	-	expression tag	UNP P47735
A	650	GLY	-	expression tag	UNP P47735
A	651	GLY	-	expression tag	UNP P47735
A	652	SER	-	expression tag	UNP P47735
A	653	ALA	-	expression tag	UNP P47735
A	654	TRP	-	expression tag	UNP P47735
A	655	SER	-	expression tag	UNP P47735
A	656	HIS	-	expression tag	UNP P47735
A	657	PRO	-	expression tag	UNP P47735
A	658	GLN	-	expression tag	UNP P47735
A	659	PHE	-	expression tag	UNP P47735
A	660	GLU	-	expression tag	UNP P47735
A	661	LYS	-	expression tag	UNP P47735
A	662	GLY	-	expression tag	UNP P47735
A	663	ALA	-	expression tag	UNP P47735
A	664	HIS	-	expression tag	UNP P47735
A	665	HIS	-	expression tag	UNP P47735
A	666	HIS	-	expression tag	UNP P47735
A	667	HIS	-	expression tag	UNP P47735
A	668	HIS	-	expression tag	UNP P47735
A	669	HIS	-	expression tag	UNP P47735
A	670	HIS	-	expression tag	UNP P47735
A	671	HIS	-	expression tag	UNP P47735
A	672	HIS	-	expression tag	UNP P47735

- Molecule 2 is a protein called Protein IDA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	0	0	0
			112	71	21	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	56	TYR	GLY	engineered mutation	UNP Q8LAD7

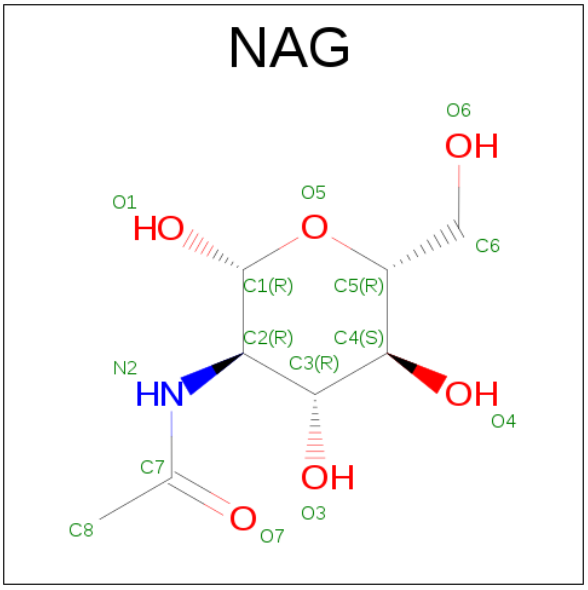
- Molecule 3 is a protein called Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	186	Total	C	N	O	S	0	1	0
			1422	897	241	279	5			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	expression tag	UNP Q94AG2
C	21	SER	-	expression tag	UNP Q94AG2
C	22	SER	-	expression tag	UNP Q94AG2
C	23	MET	-	expression tag	UNP Q94AG2
C	115	ASP	ASN	engineered mutation	UNP Q94AG2
C	163	GLN	ASN	engineered mutation	UNP Q94AG2
C	214	LEU	-	expression tag	UNP Q94AG2
C	215	GLU	-	expression tag	UNP Q94AG2
C	216	ASN	-	expression tag	UNP Q94AG2
C	217	LEU	-	expression tag	UNP Q94AG2
C	218	TYR	-	expression tag	UNP Q94AG2
C	219	PHE	-	expression tag	UNP Q94AG2
C	220	GLN	-	expression tag	UNP Q94AG2

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



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

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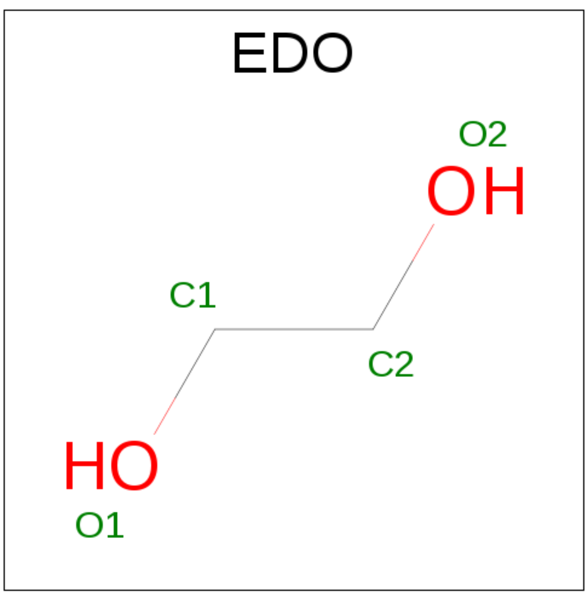
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

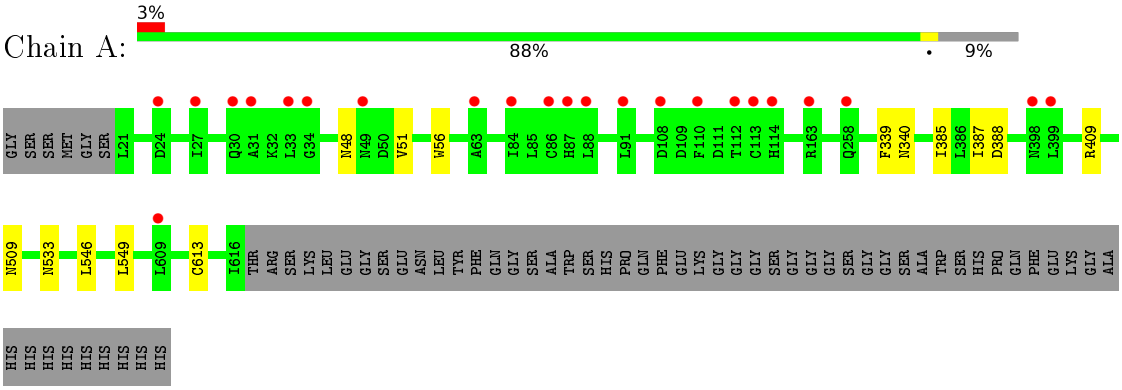
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	89	Total O 89 89	0	0
6	B	6	Total O 6 6	0	0
6	C	40	Total O 40 40	0	0

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

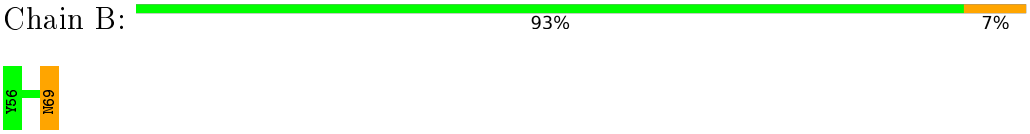
- Molecule 1: Receptor-like protein kinase 5

Chain A:



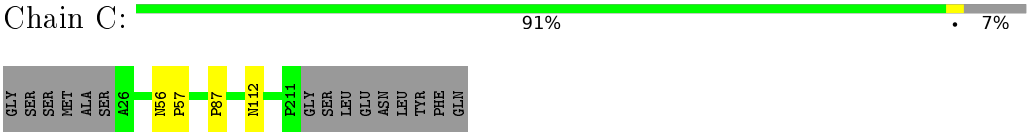
- Molecule 2: Protein IDA

Chain B:



- Molecule 3: Somatic embryogenesis receptor kinase 1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.51Å 100.46Å 142.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.43 47.38 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.38-2.43) 99.4 (47.38-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.193 , 0.234 0.197 , 0.233	Depositor DCC
R_{free} test set	2050 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: HYP, NAG, EDO

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	0.43	0/4630	0.64	0/6293
2	B	0.50	0/107	0.74	0/143
3	C	0.44	0/1454	0.68	0/1993
All	All	0.43	0/6191	0.65	0/8429

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4543	0	4559	6	0
2	B	112	0	109	1	0
3	C	1422	0	1406	2	0
4	A	140	0	126	0	0
4	C	28	0	26	0	0
5	A	8	0	12	0	0
6	A	89	0	0	0	0
6	B	6	0	0	0	0
6	C	40	0	0	0	0
All	All	6388	0	6238	8	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 1.

All (8) 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:387:ILE:HD11	1:A:409:ARG:HB3	1.73	0.71
1:A:509:ASN:HB2	1:A:533:ASN:HD21	1.67	0.59
1:A:546:LEU:HD12	1:A:549:LEU:HD22	1.98	0.46
1:A:51:VAL:HG23	1:A:56:TRP:HE1	1.82	0.45
3:C:87:PRO:HB2	3:C:112:ASN:HD21	1.84	0.43
3:C:56:ASN:HB2	3:C:57:PRO:HD2	2.01	0.42
1:A:385:ILE:HD13	2:B:69:ASN:ND2	2.36	0.40
1:A:339:PHE:HD1	1:A:340:ASN:HD22	1.68	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	595/658 (90%)	555 (93%)	39 (7%)	1 (0%)	52	64
2	B	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
3	C	185/201 (92%)	182 (98%)	3 (2%)	0	100	100
All	All	791/873 (91%)	747 (94%)	43 (5%)	1 (0%)	56	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASN

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	526/581 (90%)	524 (100%)	2 (0%)	93 96
2	B	12/12 (100%)	11 (92%)	1 (8%)	14 17
3	C	170/182 (93%)	170 (100%)	0	100 100
All	All	708/775 (91%)	705 (100%)	3 (0%)	93 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	ASP
1	A	613	CYS
2	B	69	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	533	ASN
1	A	569	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	HYP	B	64	2	6,8,9	0.97	1 (16%)	5,10,12	2.19	2 (40%)

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	HYP	B	64	2	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	64	HYP	CB-CA	-2.25	1.49	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	64	HYP	O-C-CA	-3.18	117.01	125.69
2	B	64	HYP	CB-CG-CD	3.46	107.31	103.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

14 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	1,4	14,14,15	0.28	0	15,19,21	0.79	0
4	NAG	A	702	4	14,14,15	0.52	0	15,19,21	1.79	3 (20%)
4	NAG	A	703	1	14,14,15	0.47	0	15,19,21	1.69	1 (6%)
4	NAG	A	704	1,4	14,14,15	0.45	0	15,19,21	0.91	0
4	NAG	A	705	4	14,14,15	0.65	0	15,19,21	1.14	2 (13%)
4	NAG	A	706	1,4	14,14,15	0.31	0	15,19,21	1.17	1 (6%)
4	NAG	A	707	4	14,14,15	0.31	0	15,19,21	0.95	1 (6%)
4	NAG	A	708	1	14,14,15	0.50	0	15,19,21	1.54	3 (20%)
4	NAG	A	709	1,4	14,14,15	0.33	0	15,19,21	0.80	0
4	NAG	A	710	4	14,14,15	0.50	0	15,19,21	1.11	2 (13%)
5	EDO	A	711	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	A	712	-	3,3,3	0.49	0	2,2,2	0.34	0
4	NAG	C	301	3	14,14,15	0.46	0	15,19,21	0.93	1 (6%)
4	NAG	C	302	3	14,14,15	0.48	0	15,19,21	1.19	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	702	4	-	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	4	-	0/6/23/26	0/1/1/1
4	NAG	A	706	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	707	4	-	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	710	4	-	0/6/23/26	0/1/1/1
5	EDO	A	711	-	-	0/1/1/1	0/0/0/0
5	EDO	A	712	-	-	0/1/1/1	0/0/0/0
4	NAG	C	301	3	-	0/6/23/26	0/1/1/1
4	NAG	C	302	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	302	NAG	C4-C3-C2	-2.34	107.71	111.34
4	A	708	NAG	C3-C4-C5	-2.24	106.24	110.23
4	A	705	NAG	O3-C3-C4	-2.15	105.50	110.36
4	A	708	NAG	O5-C5-C6	2.09	111.82	107.34
4	A	710	NAG	C3-C4-C5	2.19	114.14	110.23
4	A	705	NAG	C2-N2-C7	2.24	126.02	123.11
4	A	707	NAG	C1-O5-C5	2.26	115.46	112.14
4	A	702	NAG	C2-N2-C7	2.30	126.10	123.11
4	A	702	NAG	C8-C7-N2	2.45	120.79	116.10
4	C	302	NAG	C1-O5-C5	2.64	116.03	112.14
4	A	710	NAG	C4-C3-C2	2.98	115.96	111.34
4	C	301	NAG	C1-O5-C5	3.11	116.71	112.14
4	A	708	NAG	C1-O5-C5	4.20	118.31	112.14
4	A	706	NAG	C1-O5-C5	4.28	118.44	112.14
4	A	702	NAG	C1-O5-C5	4.83	119.24	112.14
4	A	703	NAG	C1-O5-C5	5.55	120.30	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	596/658 (90%)	0.31	23 (3%) 43 42	37, 61, 91, 129	0
2	B	13/14 (92%)	0.14	0 100 100	43, 47, 65, 71	0
3	C	186/201 (92%)	-0.01	0 100 100	36, 54, 77, 103	0
All	All	795/873 (91%)	0.23	23 (2%) 55 54	36, 59, 89, 129	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ILE	5.3
1	A	63	ALA	4.2
1	A	86	CYS	4.1
1	A	49	ASN	4.0
1	A	27	ILE	3.6
1	A	91	LEU	3.6
1	A	34	GLY	3.2
1	A	88	LEU	3.2
1	A	87	HIS	3.2
1	A	31	ALA	2.9
1	A	609	LEU	2.9
1	A	24	ASP	2.9
1	A	114	HIS	2.8
1	A	398	ASN	2.7
1	A	110	PHE	2.6
1	A	108	ASP	2.6
1	A	113	CYS	2.5
1	A	30	GLN	2.4
1	A	112	THR	2.3
1	A	33	LEU	2.3
1	A	399	LEU	2.1
1	A	258	GLN	2.1
1	A	163	ARG	2.0

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^{th} 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
2	HYP	B	64	8/9	0.97	0.14	-	40,43,44,46	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^{th} 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
5	EDO	A	712	4/4	0.83	0.28	4.73	73,73,74,74	0
4	NAG	A	709	14/15	0.94	0.15	0.77	57,64,69,77	0
4	NAG	A	706	14/15	0.96	0.20	-0.56	51,54,60,70	0
4	NAG	A	701	14/15	0.94	0.15	-0.94	59,65,73,82	0
4	NAG	A	704	14/15	0.94	0.13	-1.01	58,67,70,75	0
5	EDO	A	711	4/4	0.83	0.23	-	69,70,72,72	0
4	NAG	A	710	14/15	0.86	0.21	-	80,86,88,90	0
4	NAG	A	705	14/15	0.88	0.15	-	78,86,92,92	0
4	NAG	A	703	14/15	0.76	0.26	-	81,90,92,94	0
4	NAG	A	702	14/15	0.90	0.31	-	89,92,97,98	0
4	NAG	C	302	14/15	0.90	0.12	-	63,68,76,81	0
4	NAG	C	301	14/15	0.91	0.12	-	52,59,62,63	0
4	NAG	A	708	14/15	0.81	0.21	-	78,88,92,96	0
4	NAG	A	707	14/15	0.85	0.20	-	72,81,88,89	0

6.5 Other polymers (i)

There are no such residues in this entry.