



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 06:12 AM GMT

PDB ID : 3F8S
Title : Crystal structure of dipeptidyl peptidase IV in complex with inhibitor
Authors : Ammirati, M.J.; Liu, S.; Piotrowski, D.W.
Deposited on : 2008-11-13
Resolution : 2.43 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

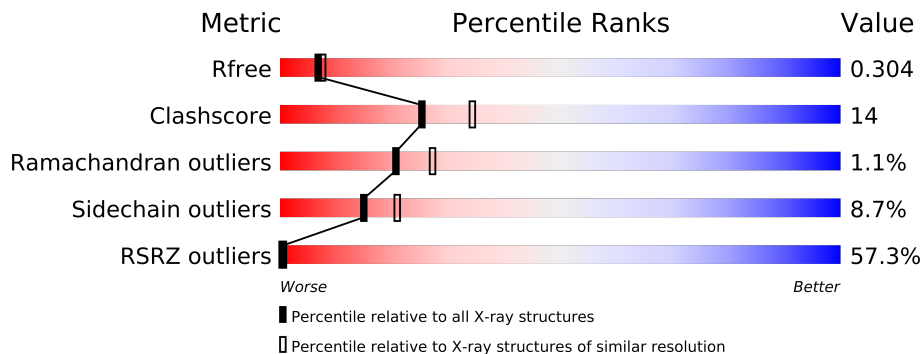
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2989 (2.48-2.40)
Clashscore	79885	3698 (2.48-2.40)
Ramachandran outliers	78287	3639 (2.48-2.40)
Sidechain outliers	78261	3640 (2.48-2.40)
RSRZ outliers	66119	2993 (2.48-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	748	
1	B	748	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	B	800	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12132 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	EXPRESSION TAG	UNP P27487
A	768	VAL	-	EXPRESSION TAG	UNP P27487
A	769	PRO	-	EXPRESSION TAG	UNP P27487
A	770	ARG	-	EXPRESSION TAG	UNP P27487
A	771	GLY	-	EXPRESSION TAG	UNP P27487
A	772	SER	-	EXPRESSION TAG	UNP P27487
A	773	HIS	-	EXPRESSION TAG	UNP P27487
A	774	HIS	-	EXPRESSION TAG	UNP P27487
A	775	HIS	-	EXPRESSION TAG	UNP P27487
A	776	HIS	-	EXPRESSION TAG	UNP P27487
A	777	HIS	-	EXPRESSION TAG	UNP P27487
A	778	HIS	-	EXPRESSION TAG	UNP P27487
B	767	LEU	-	EXPRESSION TAG	UNP P27487
B	768	VAL	-	EXPRESSION TAG	UNP P27487
B	769	PRO	-	EXPRESSION TAG	UNP P27487
B	770	ARG	-	EXPRESSION TAG	UNP P27487
B	771	GLY	-	EXPRESSION TAG	UNP P27487
B	772	SER	-	EXPRESSION TAG	UNP P27487
B	773	HIS	-	EXPRESSION TAG	UNP P27487
B	774	HIS	-	EXPRESSION TAG	UNP P27487
B	775	HIS	-	EXPRESSION TAG	UNP P27487
B	776	HIS	-	EXPRESSION TAG	UNP P27487
B	777	HIS	-	EXPRESSION TAG	UNP P27487
B	778	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

There are 48 discrepancies between the modelled and reference sequences:

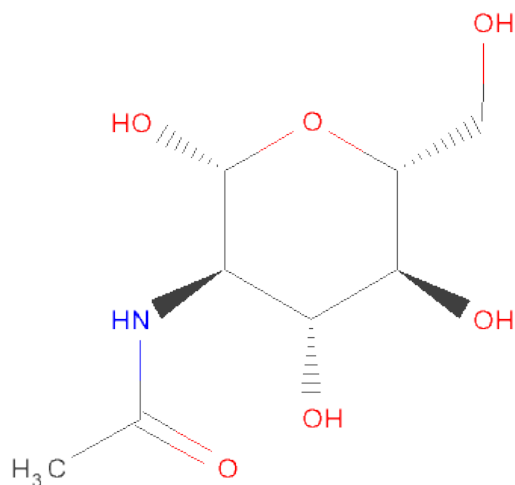
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	EXPRESSION TAG	UNP P27487
A	768	VAL	-	EXPRESSION TAG	UNP P27487
A	769	PRO	-	EXPRESSION TAG	UNP P27487
A	770	ARG	-	EXPRESSION TAG	UNP P27487
A	771	GLY	-	EXPRESSION TAG	UNP P27487
A	772	SER	-	EXPRESSION TAG	UNP P27487
A	773	HIS	-	EXPRESSION TAG	UNP P27487
A	774	HIS	-	EXPRESSION TAG	UNP P27487
A	775	HIS	-	EXPRESSION TAG	UNP P27487
A	776	HIS	-	EXPRESSION TAG	UNP P27487
A	777	HIS	-	EXPRESSION TAG	UNP P27487
A	778	HIS	-	EXPRESSION TAG	UNP P27487
A	767	LEU	-	EXPRESSION TAG	UNP P27487
A	768	VAL	-	EXPRESSION TAG	UNP P27487
A	769	PRO	-	EXPRESSION TAG	UNP P27487
A	770	ARG	-	EXPRESSION TAG	UNP P27487
A	771	GLY	-	EXPRESSION TAG	UNP P27487
A	772	SER	-	EXPRESSION TAG	UNP P27487
A	773	HIS	-	EXPRESSION TAG	UNP P27487
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A	777	HIS	-	EXPRESSION TAG	UNP P27487
A	778	HIS	-	EXPRESSION TAG	UNP P27487
B	767	LEU	-	EXPRESSION TAG	UNP P27487
B	768	VAL	-	EXPRESSION TAG	UNP P27487
B	769	PRO	-	EXPRESSION TAG	UNP P27487
B	770	ARG	-	EXPRESSION TAG	UNP P27487
B	771	GLY	-	EXPRESSION TAG	UNP P27487
B	772	SER	-	EXPRESSION TAG	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	773	HIS	-	EXPRESSION TAG	UNP P27487
B	774	HIS	-	EXPRESSION TAG	UNP P27487
B	775	HIS	-	EXPRESSION TAG	UNP P27487
B	776	HIS	-	EXPRESSION TAG	UNP P27487
B	777	HIS	-	EXPRESSION TAG	UNP P27487
B	778	HIS	-	EXPRESSION TAG	UNP P27487
B	767	LEU	-	EXPRESSION TAG	UNP P27487
B	768	VAL	-	EXPRESSION TAG	UNP P27487
B	769	PRO	-	EXPRESSION TAG	UNP P27487
B	770	ARG	-	EXPRESSION TAG	UNP P27487
B	771	GLY	-	EXPRESSION TAG	UNP P27487
B	772	SER	-	EXPRESSION TAG	UNP P27487
B	773	HIS	-	EXPRESSION TAG	UNP P27487
B	774	HIS	-	EXPRESSION TAG	UNP P27487
B	775	HIS	-	EXPRESSION TAG	UNP P27487
B	776	HIS	-	EXPRESSION TAG	UNP P27487
B	777	HIS	-	EXPRESSION TAG	UNP P27487
B	778	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



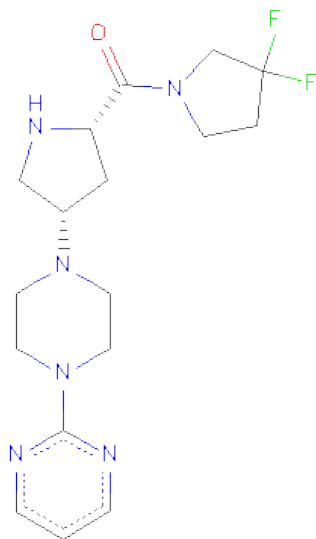
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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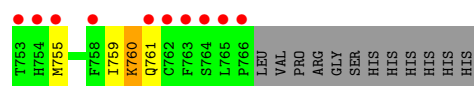
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-(4-((3S,5S)-5-[(3,3-DIFLUOROPYRROLIDIN-1-YL)CARBONYL]PYRROLIDIN-3-YL)PIPERAZIN-1-YL)PYRIMIDINE (three-letter code: PF2) (formula: C₁₇H₂₄F₂N₆O).

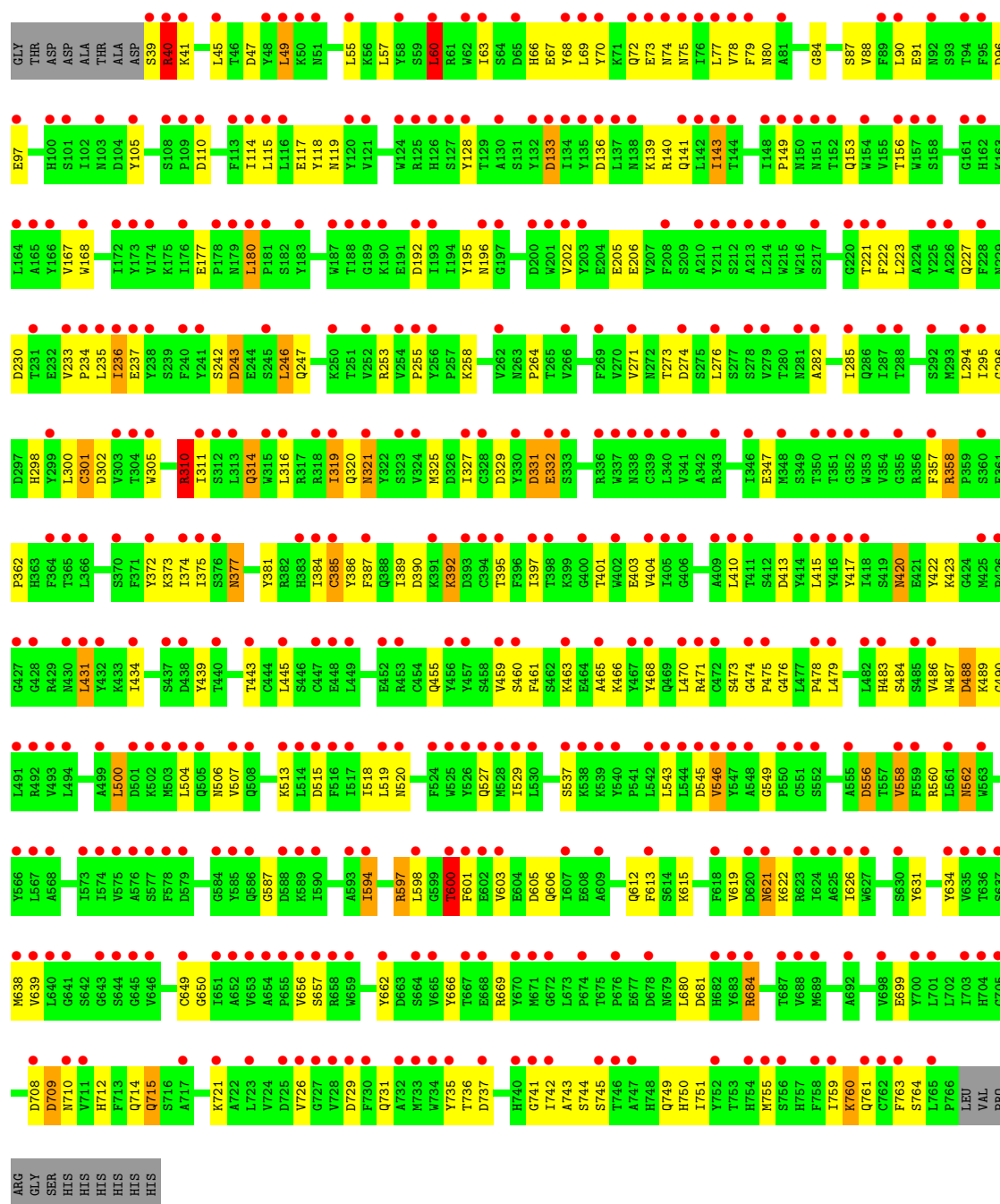


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	17	2	6	1		
4	B	1	Total	C	F	N	O	0	0
			26	17	2	6	1		



● Molecule 1: Dipeptidyl peptidase 4

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.43Å 67.14Å 421.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.43 46.57 – 2.43	Depositor EDS
% Data completeness (in resolution range)	47.8 (50.00-2.43) 47.9 (46.57-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.243 , 0.295 0.262 , 0.304	Depositor DCC
R_{free} test set	1685 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	1.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.2	EDS
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34235 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	12132	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PF2, NAG

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	0.57	0/6135	0.82	25/8344 (0.3%)
1	B	0.59	0/6135	0.84	22/8344 (0.3%)
All	All	0.58	0/12270	0.83	47/16688 (0.3%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	ARG	NE-CZ-NH1	-20.39	110.11	120.30
1	A	310	ARG	NE-CZ-NH2	-18.70	110.95	120.30
1	B	310	ARG	NE-CZ-NH2	15.96	128.28	120.30
1	A	310	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	B	310	ARG	CD-NE-CZ	9.78	137.29	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	310	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5963	0	5682	157	0
1	B	5963	0	5682	166	1
2	A	56	0	50	0	0
2	B	56	0	50	0	0
3	A	14	0	13	0	0
3	B	28	0	26	10	0
4	A	26	0	24	4	0
4	B	26	0	24	12	0
All	All	12132	0	11551	324	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 324 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:321:ASN:OD1	3:B:800:NAG:C1	2.04	1.06
3:B:799:NAG:H3	3:B:799:NAG:H83	1.41	1.01
1:B:321:ASN:CG	3:B:800:NAG:C1	2.33	0.97
1:A:470:LEU:HD12	1:A:483:HIS:HE1	1.30	0.96
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.04	0.93

All (1) 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	Distance(Å)	Clash(Å)
1:B:392:LYS:CE	1:B:506:ASN:OD1[1_545]	2.08	0.12

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	726/748 (97%)	667 (92%)	51 (7%)	8 (1%)	21	27
1	B	726/748 (97%)	669 (92%)	49 (7%)	8 (1%)	21	27
All	All	1452/1496 (97%)	1336 (92%)	100 (7%)	16 (1%)	21	27

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	140	ARG
1	A	488	ASP
1	B	140	ARG
1	B	488	ASP

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	653/669 (98%)	595 (91%)	58 (9%)	14	20
1	B	653/669 (98%)	597 (91%)	56 (9%)	15	21
All	All	1306/1338 (98%)	1192 (91%)	114 (9%)	15	21

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	710	ASN
1	B	63	ILE
1	B	621	ASN
1	A	721	LYS

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Mol	Chain	Res	Type
1	A	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	715	GLN
1	B	263	ASN
1	B	710	ASN
1	A	750	HIS
1	B	72	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

8 carbohydrates 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	NAG	A	794	1,2	12,14,15	0.72	0	15,19,21	1.37	5 (33%)
2	NAG	A	797	2	12,14,15	0.52	0	15,19,21	2.07	2 (13%)
2	NAG	A	800	1,2	12,14,15	0.65	0	15,19,21	2.08	5 (33%)
2	NAG	A	801	2	12,14,15	0.57	0	15,19,21	1.12	2 (13%)
2	NAG	B	794	1,2	12,14,15	0.67	0	15,19,21	0.73	0
2	NAG	B	796	1,2	12,14,15	0.68	0	15,19,21	2.08	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	797	2	12,14,15	0.56	0	15,19,21	1.46	3 (20%)
2	NAG	B	798	2	12,14,15	0.54	0	15,19,21	1.11	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
2	NAG	A	794	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	797	2	-	0/6/23/26	0/1/1/1
2	NAG	A	800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	801	2	-	0/6/23/26	0/1/1/1
2	NAG	B	794	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	796	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	797	2	-	0/6/23/26	0/1/1/1
2	NAG	B	798	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	797	NAG	O5-C5-C4	6.52	118.93	110.65
2	B	796	NAG	O5-C5-C6	6.35	113.64	106.98
2	A	800	NAG	C3-C2-N2	-5.82	102.90	111.76
2	B	797	NAG	C3-C2-N2	-3.68	106.15	111.76
2	A	797	NAG	C3-C4-C5	2.88	115.34	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

5 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	796	1	12,14,15	0.69	0	15,19,21	1.16	1 (6%)
4	PF2	A	900	-	29,29,29	1.49	2 (6%)	42,42,42	2.35	19 (45%)
3	NAG	B	799	1	12,14,15	0.83	0	15,19,21	2.42	3 (20%)
3	NAG	B	800	-	12,14,15	0.81	1 (8%)	15,19,21	1.01	1 (6%)
4	PF2	B	900	-	29,29,29	1.38	3 (10%)	42,42,42	2.09	15 (35%)

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	796	1	-	0/6/23/26	0/1/1/1
4	PF2	A	900	-	-	0/16/46/46	0/4/4/4
3	NAG	B	799	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	B	800	-	-	0/6/23/26	0/1/1/1
4	PF2	B	900	-	-	0/16/46/46	1/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	PF2	F25-C11	-5.77	1.30	1.37
4	A	900	PF2	F25-C11	-4.87	1.31	1.37
4	A	900	PF2	F26-C11	-4.81	1.31	1.37
4	B	900	PF2	F26-C11	-3.00	1.34	1.37
3	B	800	NAG	O5-C5	-2.07	1.41	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	799	NAG	O5-C5-C6	6.87	114.19	106.98
4	A	900	PF2	C15-N16-C17	5.65	123.28	111.67
4	B	900	PF2	C15-N16-C17	5.25	122.47	111.67
4	B	900	PF2	O7-C6-N8	4.89	127.48	121.65
4	A	900	PF2	C24-N23-C19	4.78	121.85	115.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	799	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	799	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	900	PF2	C14-C15-C17-C18-N13-N16

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	728/748 (97%)	2.42	435 (59%) 0 0	72, 84, 97, 104	0
1	B	728/748 (97%)	2.35	405 (55%) 0 0	72, 84, 97, 104	0
All	All	1456/1496 (97%)	2.39	840 (57%) 0 0	72, 84, 97, 104	0

The worst 5 of 840 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	11.9
1	B	92	ASN	11.1
1	A	587	GLY	8.6
1	A	98	PHE	8.4
1	A	183	TYR	8.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	798	14/15	0.39	1.46	114,117,119,119	0
2	NAG	B	797	14/15	0.35	0.76	91,93,96,96	0
2	NAG	A	800	14/15	0.35	-0.08	103,106,110,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	796	14/15	0.28	-0.14	89,93,100,108	0
2	NAG	A	801	14/15	0.24	-0.60	117,120,121,122	0
2	NAG	A	797	14/15	0.28	-0.68	113,115,116,116	0
2	NAG	A	794	14/15	0.22	-1.23	97,101,104,109	0
2	NAG	B	794	14/15	0.20	-1.36	78,83,89,89	0

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	800	14/15	0.47	3.50	108,109,110,111	0
4	PF2	A	900	26/26	0.32	0.65	73,77,79,81	0
4	PF2	B	900	26/26	0.32	-0.13	71,73,78,78	0
3	NAG	A	796	14/15	0.24	-0.92	85,89,92,92	0
3	NAG	B	799	14/15	0.20	-1.16	100,104,105,106	0

6.5 Other polymers ⓘ

There are no such residues in this entry.