



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:35 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 X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

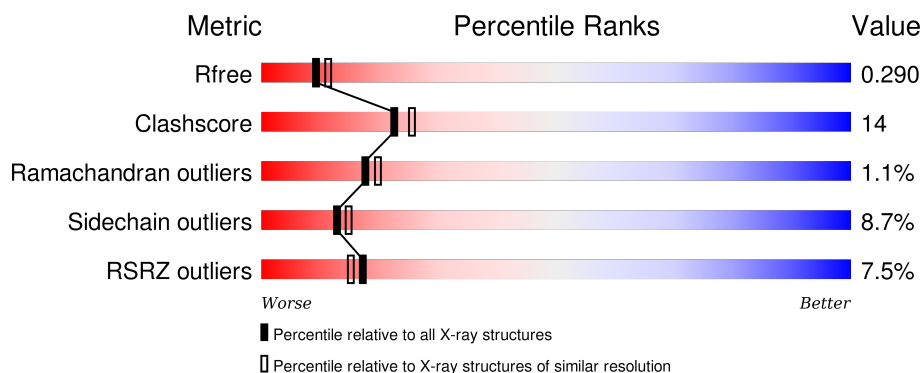
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	748	<div> <div>8%</div> <div>66%</div> <div>26%</div> <div>5% . .</div> </div>
1	B	748	<div> <div>7%</div> <div>66%</div> <div>27%</div> <div>. . .</div> </div>

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
3	NAG	B	799	X	-	-	-
4	PF2	B	900	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12132 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 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			

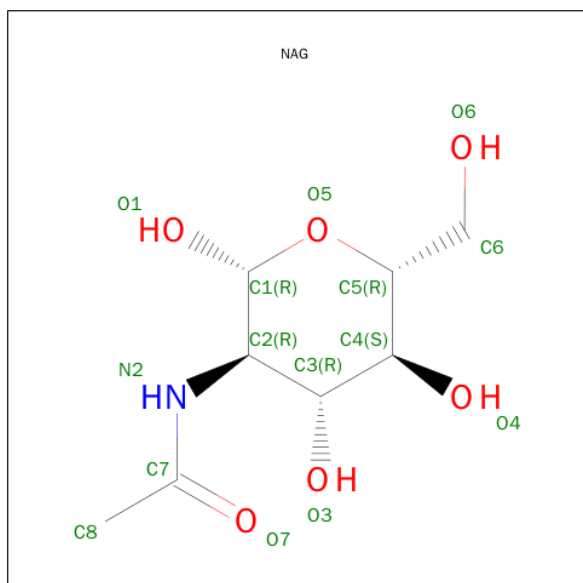
There are 24 discrepancies between the modelled and reference sequences:

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).

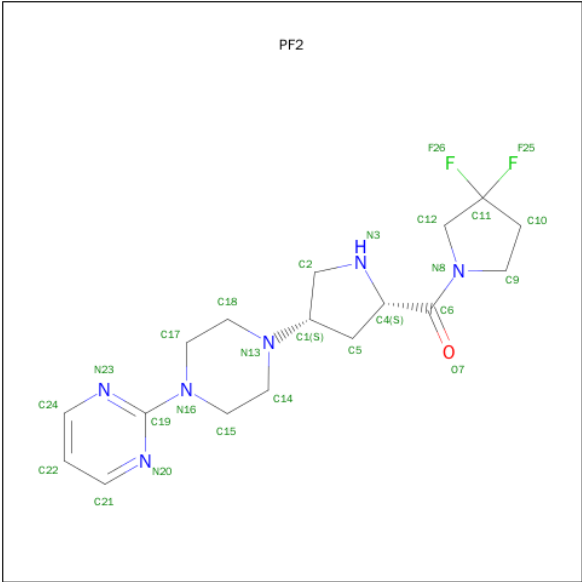
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- 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		
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:  $C_{17}H_{24}F_2N_6O$ ).

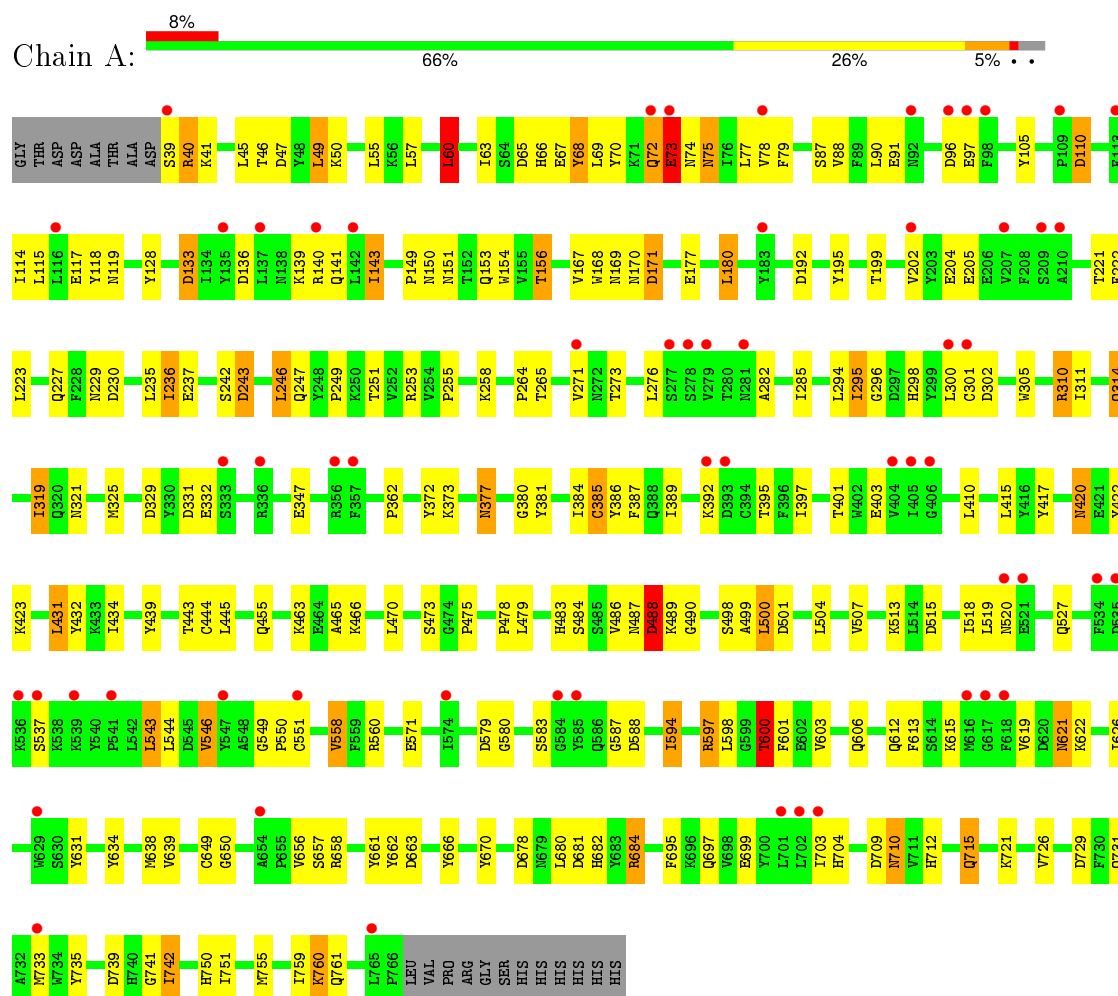


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	17	2	6	1		
4	B	1	Total	C	F	N	O	0	0
			26	17	2	6	1		

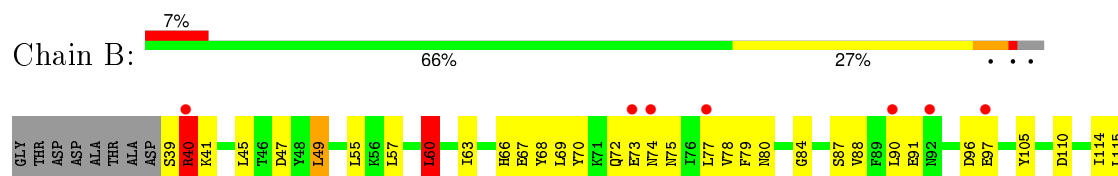
### 3 Residue-property plots

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: Dipeptidyl peptidase 4



#### • Molecule 1: Dipeptidyl peptidase 4



I751	I755	I759	K760	Q762	F763	S764	L765	P766	LEU	VAL	PRO	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS																															
V634	M638	V639	C644	L645	Q455	V459	S460	F461	S462	K463	E464	K465	K466	Y467	Y468	Q469	L470	R471	C472	S473	G474	P475	G476	L477	P478	L479	H483	S484	S485	V486	M487	D488	K489	G490	L500	D501	K502	M503	L504	Q505	N506	V507	K513	L514	D515	I518	L519	N520	Q527	M528	I529
S537	R538	K539	Y540	L543	D545	V546	Y547	A548	G549	P550	C551	S552	Q553	D556	T557	V558	F559	R560	N561	N562	I574	Y585	Q586	G587	I594	R597	L598	G599	T600	P601	E602	V603	D604	D605	Q606	Q612	F613	S614	K615	P618	V619	D620	M621	K622	I626	M629	S630	Y631			
Y439	T443	C444	L445	Q455	V459	S460	F461	S462	K463	E464	K465	K466	Y467	Y468	Q469	L470	R471	C472	S473	G474	P475	G476	L477	P478	L479	H483	S484	S485	V486	M487	D488	K489	G490	L500	D501	K502	M503	L504	Q505	N506	V507	K513	L514	D515	I518	L519	N520	Q527	M528	I529	
L340	V341	E347	G355	R356	F357	R358	P359	P362	Y372	K373	I374	I375	S376	N377	Y381	I384	C385	Y386	F387	Q388	I389	D390	K391	K392	D393	C394	T395	F396	G397	T401	M402	E403	V404	L410	D413	Y414	L415	Y416	Y417	N420	E421	Y422	K423	L431	I434						
S242	D243	L246	Q247	R253	Y254	P255	K258	P264	V271	N272	I273	D274	S275	L276	Y279	T280	N281	A282	I285	L294	I295	G296	D297	H298	Y299	L300	F396	G301	D302	W305	E206	R310	I311	Q314	W315	L316	I319	Q320	N321	M325	D326	I327	C328	D329	Y330	D331	E332				
L116	E117	Y118	M119	Y128	D133	L136	L137	N138	K139	R140	Q141	L142	I143	P149	Q153	T156	V167	W168	I176	E177	L180	D192	Y195	N196	V202	E205	V207	F208	S209	S212	T221	F222	L223	Q227	D230	V233	P234	L235	I236	E237											



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 47.8 (46.57-2.43)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.243 , 0.295 0.248 , 0.290	Depositor DCC
$R_{free}$ test set	1684 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	1.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 81.3	EDS
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34235 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 14.

The worst 5 of 324 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: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	Interatomic distance (Å)	Clash overlap (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%)	17	20
1	B	726/748 (97%)	669 (92%)	49 (7%)	8 (1%)	17	20
All	All	1452/1496 (97%)	1336 (92%)	100 (7%)	16 (1%)	17	20

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%)	12	14
1	B	653/669 (98%)	597 (91%)	56 (9%)	13	15
All	All	1306/1338 (98%)	1192 (91%)	114 (9%)	13	15

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

Mol	Chain	Res	Type
1	A	710	ASN

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Mol	Chain	Res	Type
1	B	63	ILE
1	B	621	ASN
1	A	721	LYS
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 molecules 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	14,14,15	0.56	0	15,19,21	1.26	3 (20%)
2	NAG	A	797	2	14,14,15	0.53	0	15,19,21	2.00	2 (13%)
2	NAG	A	800	1,2	14,14,15	0.81	1 (7%)	15,19,21	2.66	6 (40%)
2	NAG	A	801	2	14,14,15	0.48	0	15,19,21	1.29	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	794	1,2	14,14,15	0.78	1 (7%)	15,19,21	0.98	1 (6%)
2	NAG	B	796	1,2	14,14,15	0.60	0	15,19,21	1.45	3 (20%)
2	NAG	B	797	2	14,14,15	0.62	0	15,19,21	1.30	2 (13%)
2	NAG	B	798	2	14,14,15	0.49	0	15,19,21	1.10	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	794	NAG	O5-C1	-2.48	1.39	1.43
2	A	800	NAG	C1-C2	2.69	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	NAG	C3-C2-N2	-3.20	102.90	110.56
2	B	798	NAG	C2-N2-C7	-2.76	119.50	123.04
2	B	797	NAG	C2-N2-C7	-2.74	119.52	123.04
2	A	794	NAG	C2-N2-C7	-2.59	119.71	123.04
2	B	796	NAG	C2-N2-C7	-2.50	119.83	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	14,14,15	0.61	0	15,19,21	1.08	1 (6%)
4	PF2	A	900	-	26,29,29	1.66	2 (7%)	30,42,42	2.54	15 (50%)
3	NAG	B	799	1	14,14,15	0.69	0	15,19,21	1.81	3 (20%)
3	NAG	B	800	-	14,14,15	0.59	0	15,19,21	0.87	0
4	PF2	B	900	-	26,29,29	1.54	2 (7%)	30,42,42	2.31	13 (43%)

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	0/6/23/26	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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	PF2	F25-C11	-6.24	1.30	1.38
4	A	900	PF2	F25-C11	-5.29	1.31	1.38
4	A	900	PF2	F26-C11	-5.22	1.31	1.38
4	B	900	PF2	F26-C11	-3.32	1.34	1.38

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	PF2	F25-C11-C10	-4.26	100.92	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	799	NAG	C6-C5-C4	-4.20	102.66	113.02
4	B	900	PF2	C4-C6-N8	-4.20	112.29	118.95
4	A	900	PF2	C10-C9-N8	-3.96	100.05	103.78
4	A	900	PF2	C17-N16-C19	-3.50	116.30	121.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	799	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

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

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	900	PF2	4	0
3	B	799	NAG	4	0
3	B	800	NAG	6	0
4	B	900	PF2	12	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	728/748 (97%)	0.62	59 (8%) 15 13	72, 84, 97, 104	0
1	B	728/748 (97%)	0.58	50 (6%) 20 18	72, 84, 97, 104	0
All	All	1456/1496 (97%)	0.60	109 (7%) 17 15	72, 84, 97, 104	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	6.3
1	A	137	LEU	6.3
1	A	39	SER	5.6
1	A	278	SER	5.1
1	A	279	VAL	5.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	800	14/15	0.83	0.17	0.98	103,106,110,113	0
2	NAG	B	796	14/15	0.87	0.18	0.24	89,93,100,108	0
2	NAG	A	794	14/15	0.93	0.14	-0.87	97,101,104,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	794	14/15	0.93	0.11	-1.43	78,83,89,89	0
2	NAG	A	801	14/15	0.84	0.31	-	117,120,121,122	0
2	NAG	B	797	14/15	0.92	0.17	-	91,93,96,96	0
2	NAG	B	798	14/15	0.86	0.41	-	114,117,119,119	0
2	NAG	A	797	14/15	0.82	0.29	-	113,115,116,116	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	800	14/15	0.93	0.19	1.59	108,109,110,111	0
4	PF2	B	900	26/26	0.93	0.27	-0.05	71,73,78,78	0
3	NAG	A	796	14/15	0.89	0.18	-0.35	85,89,92,92	0
4	PF2	A	900	26/26	0.94	0.25	-0.42	73,77,79,81	0
3	NAG	B	799	14/15	0.86	0.17	-	100,104,105,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.