



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:18 PM GMT

PDB ID : 1DDX  
Title : CRYSTAL STRUCTURE OF A MIXTURE OF ARACHIDONIC ACID AND PROSTAGLANDIN BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2: PROSTAGLANDIN STRUCTURE  
Authors : Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.  
Deposited on : 1999-11-11  
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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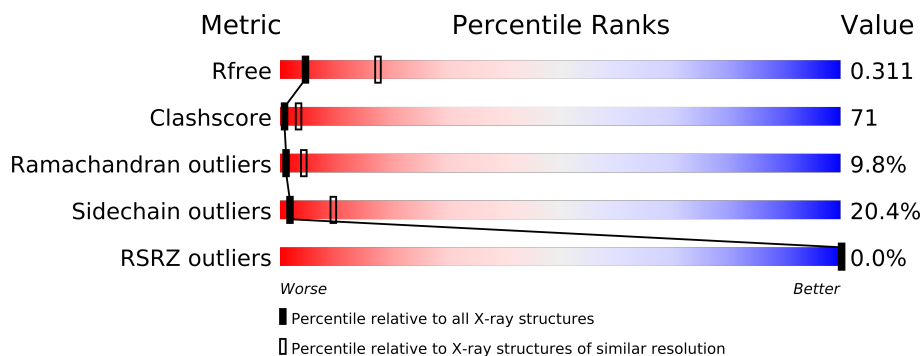
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. 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	552	
1	B	552	
1	C	552	
1	D	552	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18477 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 PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	B	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	C	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	D	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			

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

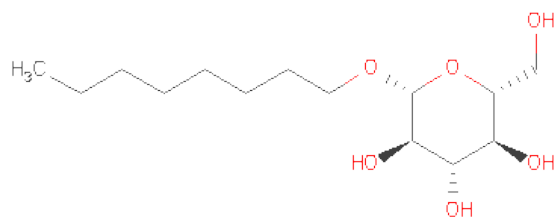
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



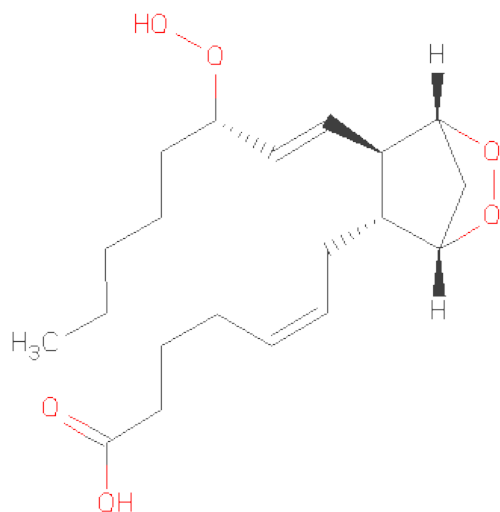
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

- Molecule 4 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is 7-[6-(3-HYDROPEROXY-OCT-1-ENYL)-2,3-DIOXA-BICYCLO[2.2.1]HEPT-5-YL]-HEPT-5-ENOICACID (three-letter code: PGX) (formula: C<sub>20</sub>H<sub>32</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	20	5		
5	B	1	Total	C	O	0	0
			25	20	5		
5	C	1	Total	C	O	0	0
			25	20	5		
5	D	1	Total	C	O	0	0
			25	20	5		

- Molecule 6 is water.

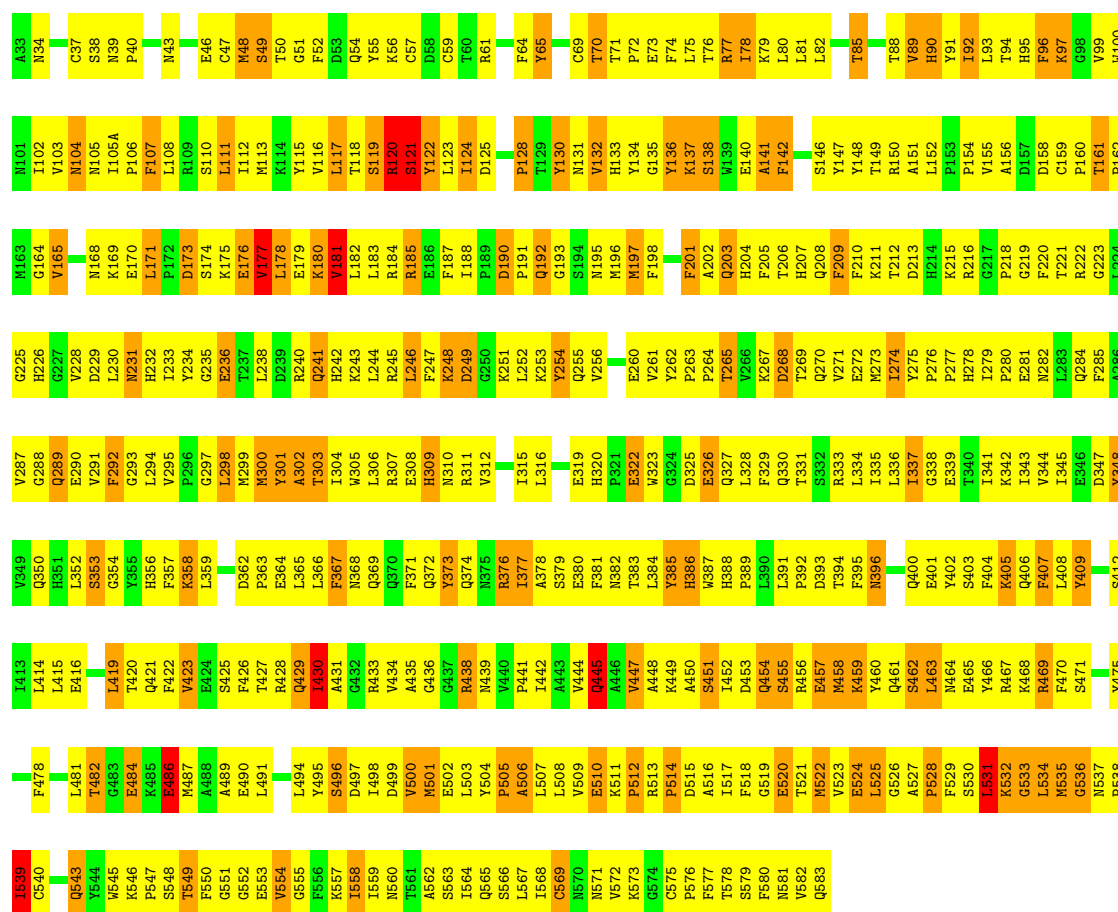
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	39	Total	O	0	0
			39	39		
6	C	46	Total	O	0	0
			46	46		
6	D	43	Total	O	0	0
			43	43		

### 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.

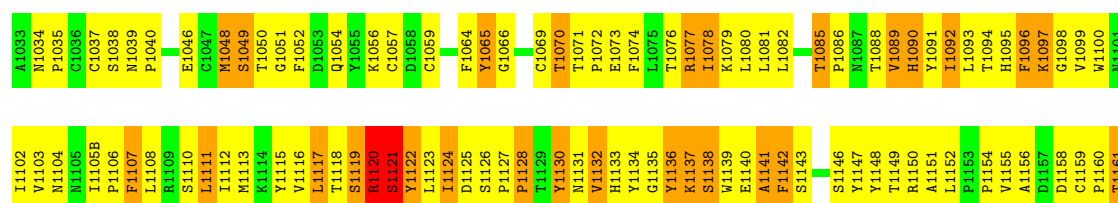
#### • Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

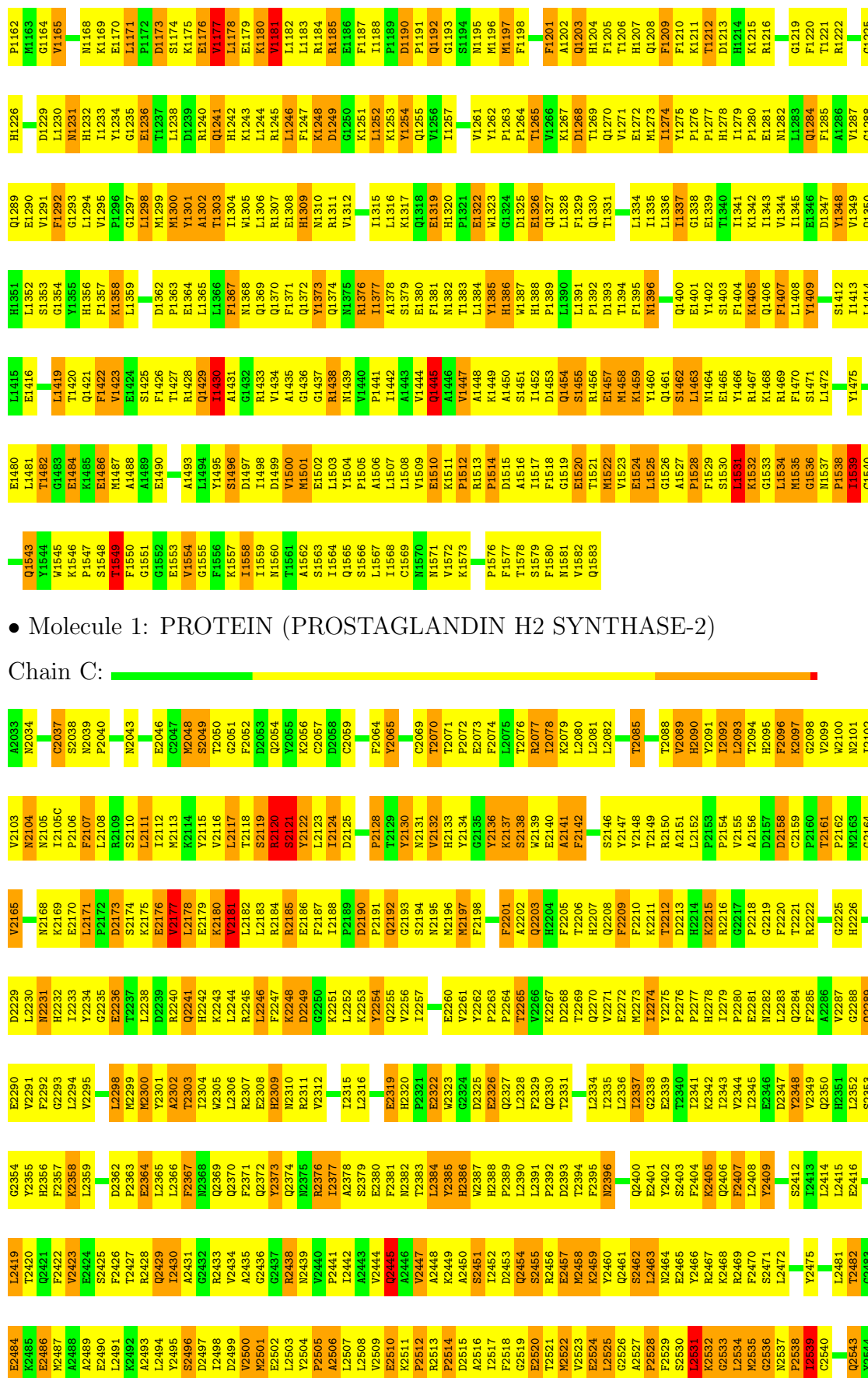
Chain A:



#### • Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

Chain B:







W2545
K2546
P2547
S2548
T2549
P2550
G2551
C2552
E2553
V2554
G2555
P2556
K2557
I2558
N2559
N2560

S2563
I2564
Q2565
S2566
L2567
I2568
C2569
N2570
N2571
V2572
K2573

P2576
T2577
S2578
S2579
N2581
V2582
Q2583

● Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

Chain D:

L3053
N3054
P3056
C3036
N3101
I3102
V3103
S3038
N3039
P3040

N3043
E3046
C5047
N3048
S3049
T3050
G3051
F3052
D3053
Q3054
Y3055
K3056
C3057
D3058
C3059

T3062
G3063
F3064
Y3065
G3066
C3069
T3070
T3071
P3072
E3073
F3074
L3075
T3076
R3077
I3078
K3079
L3080
L3081
L3082

S3085
P3086
N3087
T3088
V3089
H3090
Y3091
L3092
I3093
L3094
T3095
F3096
D3097

G3098
V3099
N3100
N3101
I3102
V3103
G3104
N3105
L3105D
F3107
L3108

L3111
I3112
M3113
G3114
Y3115
F3116
L3117
T3118
S3119
R3120
S3121
Y3122
L3123
I3124

G3125
F3126
Y3127
G3128
T3129
Y3130
N3131
V3132
H3133
Y3134
M3136
G3135
F3136
K3137
S3138
W3139
E3140
A3141
F3142
S3143

S3146
Y3147
Y3148
T3149
R3150
A3151
L3152
P3153
L3154
L3155
A3156
D3157
K3158

C3159
F3160
T3161
T3162
M3163
G3164
V3165

N3168
K3169
E3170
L3171
P3172
D3173
K3174
K3175
E3176
V3177
L3178
E3179
K3180
V3181
L3182
L3183
R3184
R3185
E3186
F3187
L3188
P3189
D3190
P3191
K3192
G3193
S3194
N3195
M3196
M3197
F3198
A3199
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P3201
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Q3203
H3204
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T3206
H3207
Q3208
F3209
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T3212
D3213
H3214
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K3216
G3217
G3219

D3220
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V3228
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L3230
N3231
H3232
L3233
Y3234
G3235
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D3249
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L3252
K3253
Y3254
Q3255
V3256
I3257

E3260
V3261
Y3262
P3263
P3264
T3265
Y3266
K3267
T3268
Q3270
V3271
E3272
K3273
I3274
Y3275
P3276
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H3278
I3279
P3280
E3281

N3282
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V3287
L3288
G3289
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L3294
V3295

L3298
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T3303
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E3308
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I3345

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T3394
F3395
N3396

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.24Å 134.80Å 122.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 36.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-3.00) 75.8 (36.19-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.267 , 0.324 0.258 , 0.311	Depositor DCC
$R_{free}$ test set	4329 reflections (10.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 26.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 45890 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	18477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.3521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities 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: NAG, PGX, BOG

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	0.45	0/4602	0.65	0/6239
1	B	0.45	0/4602	0.65	0/6239
1	C	0.45	0/4602	0.65	0/6239
1	D	0.46	0/4602	0.64	0/6239
All	All	0.45	0/18408	0.64	0/24956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4475	0	4373	650	0
1	B	4475	0	4373	653	0
1	C	4475	0	4373	663	0
1	D	4475	0	4373	668	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0
4	C	20	0	28	0	0
4	D	20	0	28	1	0
5	A	25	0	30	9	0
5	B	25	0	30	13	0
5	C	25	0	30	14	0
5	D	25	0	30	11	0
6	A	45	0	0	14	0
6	B	39	0	0	12	0
6	C	46	0	0	20	0
6	D	43	0	0	15	0
All	All	18477	0	17928	2579	0

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 71.

The worst 5 of 2579 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:3312:VAL:HA	1:D:3315:ILE:HD12	1.33	1.09
1:A:312:VAL:HA	1:A:315:ILE:HD12	1.33	1.08
1:B:1312:VAL:HA	1:B:1315:ILE:HD12	1.36	1.07
1:B:1301:TYR:HA	1:B:1304:ILE:HD12	1.37	1.07
1:A:99:VAL:HA	1:A:102:ILE:HD12	1.37	1.06

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	550/552 (100%)	374 (68%)	124 (22%)	52 (10%)	1	4
1	B	550/552 (100%)	379 (69%)	119 (22%)	52 (10%)	1	4
1	C	550/552 (100%)	372 (68%)	120 (22%)	58 (10%)	1	3
1	D	550/552 (100%)	376 (68%)	121 (22%)	53 (10%)	1	4
All	All	2200/2208 (100%)	1501 (68%)	484 (22%)	215 (10%)	1	4

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	A	176	GLU
1	A	180	LYS
1	A	348	TYR

### 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	493/493 (100%)	391 (79%)	102 (21%)	2	8
1	B	493/493 (100%)	391 (79%)	102 (21%)	2	8
1	C	493/493 (100%)	393 (80%)	100 (20%)	2	9
1	D	493/493 (100%)	394 (80%)	99 (20%)	2	10
All	All	1972/1972 (100%)	1569 (80%)	403 (20%)	2	9

5 of 403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1457	GLU
1	C	2136	TYR
1	D	3412	SER
1	B	1482	THR
1	C	2046	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1560	ASN
1	C	2327	GLN
1	D	3464	ASN
1	B	1565	GLN
1	B	1581	ASN

### 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	661	1,2	12,14,15	0.62	0	15,19,21	0.65	0
2	NAG	A	662	2	12,14,15	0.59	0	15,19,21	0.40	0
2	NAG	B	1661	1,2	12,14,15	0.81	0	15,19,21	0.70	0
2	NAG	B	1662	2	12,14,15	0.69	0	15,19,21	0.41	0
2	NAG	C	2661	1,2	12,14,15	0.58	0	15,19,21	0.69	0
2	NAG	C	2662	2	12,14,15	0.58	0	15,19,21	0.41	0
2	NAG	D	3661	1,2	12,14,15	0.68	0	15,19,21	0.66	0
2	NAG	D	3662	2	12,14,15	0.62	0	15,19,21	0.46	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
2	NAG	A	661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	662	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1662	2	-	0/6/23/26	0/1/1/1
2	NAG	C	2661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2662	2	-	0/6/23/26	0/1/1/1
2	NAG	D	3661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	3662	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

16 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	671	1	12,14,15	0.61	0	15,19,21	0.95	1 (6%)
3	NAG	A	681	1	12,14,15	0.50	0	15,19,21	0.68	0
5	PGX	A	701	-	26,26,27	1.42	3 (11%)	31,33,34	1.56	3 (9%)
4	BOG	A	702	-	20,20,20	0.87	2 (10%)	25,25,25	0.64	0
3	NAG	B	1671	1	12,14,15	0.56	0	15,19,21	0.89	0
3	NAG	B	1681	1	12,14,15	0.49	0	15,19,21	0.62	0
5	PGX	B	1701	-	26,26,27	1.42	1 (3%)	31,33,34	1.58	3 (9%)
4	BOG	B	1702	-	20,20,20	0.84	2 (10%)	25,25,25	0.65	0
3	NAG	C	2671	1	12,14,15	0.66	0	15,19,21	1.04	1 (6%)
3	NAG	C	2681	1	12,14,15	0.54	0	15,19,21	0.60	0
5	PGX	C	2701	-	26,26,27	1.38	1 (3%)	31,33,34	1.57	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BOG	C	2702	-	20,20,20	0.93	2 (10%)	25,25,25	0.63	0
3	NAG	D	3671	1	12,14,15	0.51	0	15,19,21	0.75	0
3	NAG	D	3681	1	12,14,15	0.51	0	15,19,21	0.51	0
5	PGX	D	3701	-	26,26,27	1.42	3 (11%)	31,33,34	1.54	2 (6%)
4	BOG	D	3702	-	20,20,20	0.86	2 (10%)	25,25,25	0.62	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	NAG	A	671	1	-	0/6/23/26	0/1/1/1
3	NAG	A	681	1	-	0/6/23/26	0/1/1/1
5	PGX	A	701	-	-	0/19/40/42	0/0/2/2
4	BOG	A	702	-	-	0/11/31/31	0/1/1/1
3	NAG	B	1671	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1681	1	-	0/6/23/26	0/1/1/1
5	PGX	B	1701	-	-	0/19/40/42	0/0/2/2
4	BOG	B	1702	-	-	0/11/31/31	0/1/1/1
3	NAG	C	2671	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2681	1	-	0/6/23/26	0/1/1/1
5	PGX	C	2701	-	-	0/19/40/42	0/0/2/2
4	BOG	C	2702	-	-	0/11/31/31	0/1/1/1
3	NAG	D	3671	1	-	0/6/23/26	0/1/1/1
3	NAG	D	3681	1	-	0/6/23/26	0/1/1/1
5	PGX	D	3701	-	-	0/19/40/42	0/0/2/2
4	BOG	D	3702	-	-	0/11/31/31	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1701	PGX	O4-O3	-5.70	1.24	1.46
5	D	3701	PGX	O4-O3	-5.66	1.24	1.46
5	C	2701	PGX	O4-O3	-5.65	1.24	1.46
5	A	701	PGX	O4-O3	-5.58	1.24	1.46
4	C	2702	BOG	O1-C1	2.67	1.45	1.40

The worst 5 of 14 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3701	PGX	C11-C10-C9	-5.98	85.67	103.82
5	A	701	PGX	C11-C10-C9	-5.92	85.86	103.82
5	B	1701	PGX	C11-C10-C9	-5.89	85.95	103.82
5	C	2701	PGX	C11-C10-C9	-5.88	85.99	103.82
5	B	1701	PGX	C7-C8-C9	3.52	118.68	113.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	552/552 (100%)	-0.19	0 100 100	2, 25, 52, 71	0
1	B	552/552 (100%)	-0.16	0 100 100	3, 25, 51, 70	0
1	C	552/552 (100%)	-0.21	0 100 100	2, 25, 51, 70	0
1	D	552/552 (100%)	-0.17	0 100 100	3, 25, 51, 70	0
All	All	2208/2208 (100%)	-0.18	0 100 100	2, 25, 51, 71	0

There are no RSRZ outliers to report.

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	3662	14/15	0.47	-	77,80,85,86	0
2	NAG	A	662	14/15	0.61	-	77,81,84,84	0
2	NAG	B	1662	14/15	0.47	-	78,81,84,84	0
2	NAG	C	2662	14/15	0.49	-	78,81,85,85	0
2	NAG	B	1661	14/15	0.35	-	52,60,67,74	0
2	NAG	C	2661	14/15	0.21	-	51,59,64,72	0
2	NAG	D	3661	14/15	0.37	-	51,62,66,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	661	14/15	0.36	-	52,59,65,72	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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	681	14/15	0.38	-	67,70,73,74	0
5	PGX	C	2701	25/26	0.53	-	75,79,84,84	0
3	NAG	A	671	14/15	0.19	-	2,9,25,27	0
4	BOG	D	3702	20/20	0.41	-	46,53,59,62	0
3	NAG	B	1671	14/15	0.19	-	5,10,25,26	0
4	BOG	B	1702	20/20	0.36	-	50,54,59,59	0
4	BOG	A	702	20/20	0.51	-	54,58,62,65	0
3	NAG	C	2681	14/15	0.53	-	66,69,73,73	0
3	NAG	C	2671	14/15	0.18	-	7,10,25,28	0
3	NAG	B	1681	14/15	0.32	-	66,71,73,75	0
4	BOG	C	2702	20/20	0.47	-	56,60,64,66	0
3	NAG	D	3681	14/15	0.28	-	66,70,72,73	0
5	PGX	A	701	25/26	0.48	-	73,78,86,87	0
3	NAG	D	3671	14/15	0.15	-	2,9,23,25	0
5	PGX	D	3701	25/26	0.41	-	74,78,86,87	0
5	PGX	B	1701	25/26	0.48	-	72,78,84,85	0

## 6.5 Other polymers

There are no such residues in this entry.