



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 7, 2017 – 08:11 PM EST

PDB ID : 4OTJ
Title : The complex of murine cyclooxygenase-2 with a conjugate of indomefathin and podophyllotoxin, N-{(succinylpodophyllotoxiny)but-4-yl}-2-{1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl}acetamide
Authors : Xu, S.; Uddin, M.J.; Banerjee, S.; Marnett, L.J.
Deposited on : 2014-02-13
Resolution : 2.11 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

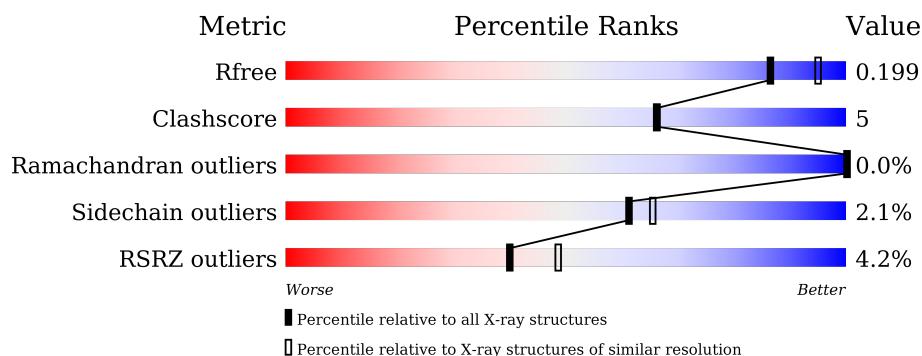
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	587	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>7% • 6%</div> </div> </div>
1	B	587	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>8% • 6%</div> </div> </div>
1	C	587	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>7% • 6%</div> </div> </div>
1	D	587	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8% • 6%</div> </div> </div>

2 Entry composition [i](#)

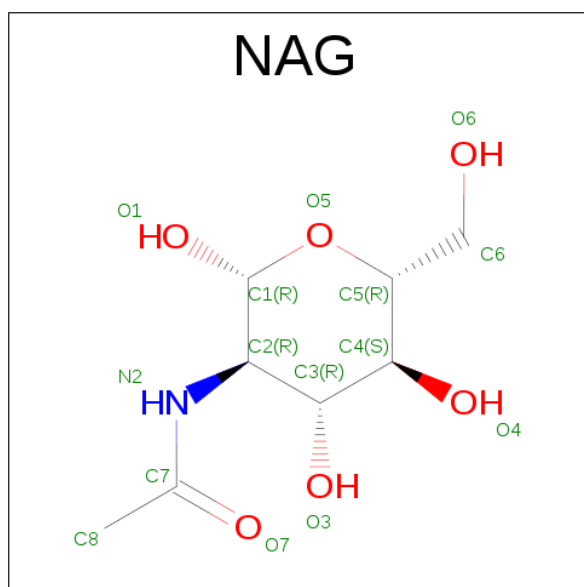
There are 7 unique types of molecules in this entry. The entry contains 20131 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	1	0
			4482	2890	753	814	25			
1	B	551	Total	C	N	O	S	0	0	0
			4465	2880	748	812	25			
1	C	552	Total	C	N	O	S	0	1	0
			4482	2890	753	814	25			
1	D	551	Total	C	N	O	S	0	1	0
			4471	2884	748	814	25			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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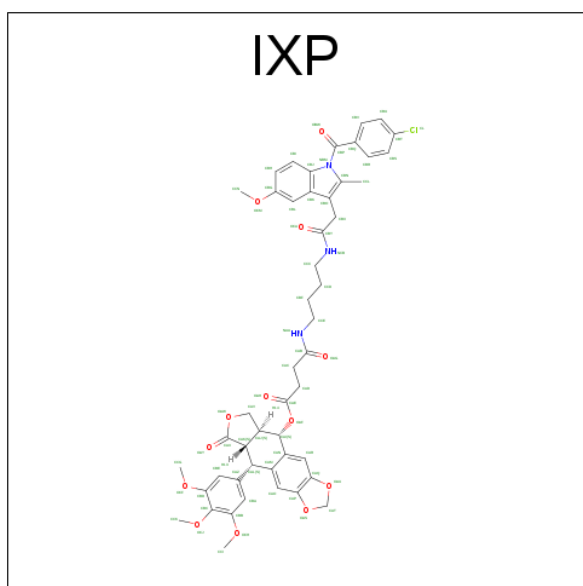
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0

- | Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 3 | A | 2 | Total
28 | C
16 | N
2 | O
10 | 0 | 0 |
| 3 | B | 2 | Total
28 | C
16 | N
2 | O
10 | 0 | 0 |
| 3 | C | 2 | Total
28 | C
16 | N
2 | O
10 | 0 | 0 |
| 3 | D | 2 | Total
28 | C
16 | N
2 | O
10 | 0 | 0 |

- # HEM

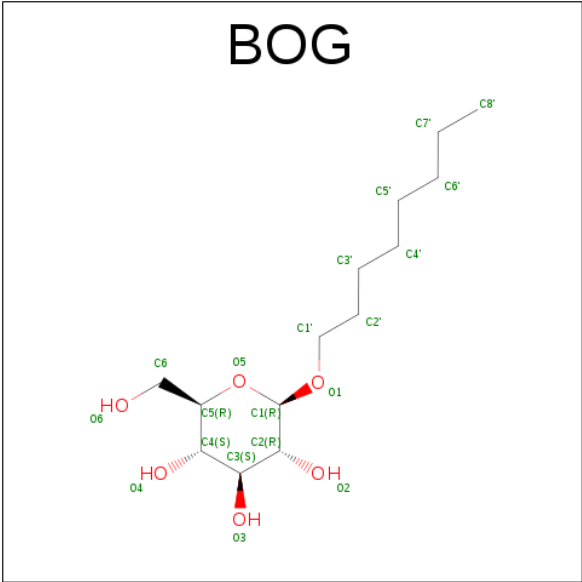
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is (5S,5AS,8AS,9S)-8-OXO-9-(3,4,5-TRIMETHOXYPHENYL)-5,5A,6,8,8A,9-H EXAHYDROFURO[3',4':6,7]NAPHTHO[2,3-D][1,3]DIOXOL-5-YL 4-{[4-({[1-(4-CHLORO BENZOYL)-5-METHOXY-2-METHYL-1H-INDOL-3-YL]ACETYL} AMINO)BUTYL]AMINO}-4-OXOBUTANOATE (three-letter code: IXP) (formula: C₄₉H₅₀ClN₃O₁₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 66	C 49	Cl 1	N 3	O 13	34	0
5	B	1	Total 66	C 49	Cl 1	N 3	O 13	36	0
5	C	1	Total 66	C 49	Cl 1	N 3	O 13	41	0
5	D	1	Total 66	C 49	Cl 1	N 3	O 13	34	0

- Molecule 6 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).

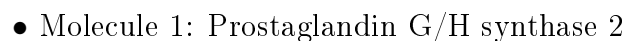


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			20	14	6		
6	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 7 is water.

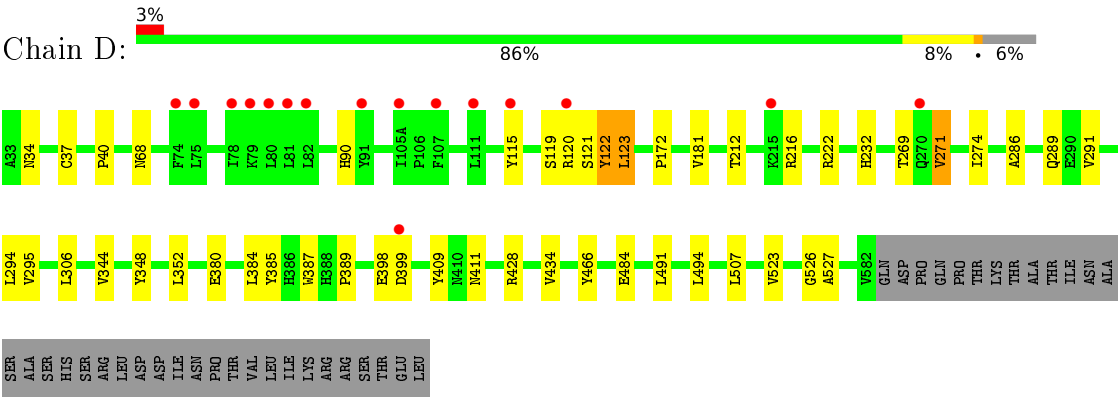
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	340	Total	O	0	0
			340	340		
7	B	336	Total	O	0	0
			336	336		
7	C	406	Total	O	0	0
			406	406		
7	D	449	Total	O	0	0
			449	449		

- Molecule 1: Prostaglandin G/H synthase 2



HIS
SER
ARG
LEU
ASP
ASP
ILE
ASN
PRO
THR
VAL
LEU
LEU
LYS
ARG
ARG
SER
THR
GLU
LEU

• Molecule 1: Prostaglandin G/H synthase 2



SER
ALA
SER
HIS
SER
ARG
LEU
ASP
ASP
ILE
ASN
PRO
THR
VAL
LEU
ILE
LYS
ARG
ARG
SER
THR
GLU
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.71Å 133.94Å 122.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.11 – 2.11 50.11 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.11-2.11) 99.6 (50.11-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.177 , 0.199 0.176 , 0.199	Depositor DCC
R_{free} test set	5122 reflections (3.02%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20131	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 45.35 % 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 1.3388e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: HEM, IXP, NAG, 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	0.33	0/4612	0.50	0/6253
1	B	0.36	0/4592	0.50	0/6227
1	C	0.34	0/4612	0.51	0/6253
1	D	0.36	0/4601	0.51	0/6239
All	All	0.35	0/18417	0.51	0/24972

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 [i](#)

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	4482	0	4386	29	0
1	B	4465	0	4365	46	0
1	C	4482	0	4386	35	0
1	D	4471	0	4371	34	0
2	A	28	0	26	2	0
2	B	28	0	26	1	0
2	C	28	0	26	2	0
2	D	28	0	26	2	0
3	A	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	25	1	0
3	C	28	0	25	1	0
3	D	28	0	25	1	0
4	A	43	0	30	2	0
4	B	43	0	30	2	0
4	C	43	0	30	2	0
4	D	43	0	30	2	0
5	A	66	0	50	7	0
5	B	66	0	50	13	0
5	C	66	0	50	7	0
5	D	66	0	50	13	0
6	B	20	0	25	4	0
6	D	20	0	25	1	0
7	A	340	0	0	7	0
7	B	336	0	0	3	0
7	C	406	0	0	7	0
7	D	449	0	0	4	0
All	All	20131	0	18082	177	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 5.

The worst 5 of 177 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:D:115:TYR:O	1:D:119:SER:HB3	1.53	1.07
1:D:523:VAL:CG2	5:D:707:IXP:H44	1.85	1.06
1:D:523:VAL:HG21	5:D:707:IXP:H44	1.36	1.06
1:A:120:ARG:NH2	5:A:706:IXP:H33	1.76	0.99
6:B:701:BOG:H1'2	6:B:701:BOG:H5'2	1.51	0.92

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	551/587 (94%)	536 (97%)	15 (3%)	0	100	100
1	B	549/587 (94%)	531 (97%)	18 (3%)	0	100	100
1	C	551/587 (94%)	535 (97%)	16 (3%)	0	100	100
1	D	550/587 (94%)	533 (97%)	16 (3%)	1 (0%)	52	52
All	All	2201/2348 (94%)	2135 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	122	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	494/525 (94%)	486 (98%)	8 (2%)	70	75
1	B	492/525 (94%)	481 (98%)	11 (2%)	60	63
1	C	494/525 (94%)	481 (97%)	13 (3%)	54	57
1	D	493/525 (94%)	483 (98%)	10 (2%)	63	67
All	All	1973/2100 (94%)	1931 (98%)	42 (2%)	61	65

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	556	PHE
1	C	123	LEU
1	D	306	LEU
1	C	79	LYS
1	C	120	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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	$\# Z > 2$
3	NAG	A	702	1,3	14,14,15	0.19	0	15,19,21	0.66	1 (6%)
3	NAG	A	703	3	14,14,15	0.41	0	15,19,21	0.39	0
3	NAG	B	703	1,3	14,14,15	0.33	0	15,19,21	0.50	0
3	NAG	B	704	3	14,14,15	0.49	0	15,19,21	0.37	0
3	NAG	C	702	1,3	14,14,15	0.15	0	15,19,21	0.56	0
3	NAG	C	703	3	14,14,15	0.63	1 (7%)	15,19,21	0.58	0
3	NAG	D	702	1,3	14,14,15	0.29	0	15,19,21	0.64	1 (6%)
3	NAG	D	703	3	14,14,15	0.49	0	15,19,21	0.36	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	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	703	3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	704	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	703	3	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	703	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	NAG	C1-C2	2.08	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	NAG	C1-O5-C5	2.05	115.15	112.14
3	A	702	NAG	C1-O5-C5	2.21	115.39	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	1	0
3	B	704	NAG	1	0
3	C	703	NAG	1	0
3	D	703	NAG	1	0

5.6 Ligand geometry

18 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
2	NAG	A	701	1	14,14,15	0.84	1 (7%)	15,19,21	1.24	1 (6%)
2	NAG	A	704	1	14,14,15	0.37	0	15,19,21	0.42	0
4	HEM	A	705	1,7	24,50,50	2.43	6 (25%)	16,82,82	1.53	3 (18%)
5	IXP	A	706	-	71,73,73	2.53	15 (21%)	93,105,105	1.85	17 (18%)
6	BOG	B	701	-	20,20,20	1.65	5 (25%)	25,25,25	1.81	7 (28%)
2	NAG	B	702	1	14,14,15	0.69	1 (7%)	15,19,21	1.16	1 (6%)
2	NAG	B	705	1	14,14,15	0.35	0	15,19,21	0.50	0
4	HEM	B	706	1,7	24,50,50	2.37	5 (20%)	16,82,82	1.77	3 (18%)
5	IXP	B	707	-	71,73,73	2.52	15 (21%)	93,105,105	1.89	18 (19%)
2	NAG	C	701	1	14,14,15	0.73	1 (7%)	15,19,21	1.08	1 (6%)
2	NAG	C	704	1	14,14,15	0.34	0	15,19,21	0.40	0
4	HEM	C	705	1,7	24,50,50	2.40	6 (25%)	16,82,82	1.76	4 (25%)
5	IXP	C	706	-	71,73,73	2.67	16 (22%)	93,105,105	2.00	22 (23%)
2	NAG	D	701	1	14,14,15	0.80	1 (7%)	15,19,21	1.21	1 (6%)
2	NAG	D	704	1	14,14,15	0.41	0	15,19,21	0.45	0
4	HEM	D	705	1,7	24,50,50	2.38	5 (20%)	16,82,82	1.67	2 (12%)
6	BOG	D	706	-	20,20,20	1.62	7 (35%)	25,25,25	1.42	1 (4%)
5	IXP	D	707	-	71,73,73	2.50	15 (21%)	93,105,105	1.84	16 (17%)

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	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	HEM	A	705	1,7	-	0/6/54/54	0/0/8/8
5	IXP	A	706	-	-	0/38/77/77	0/8/8/8
6	BOG	B	701	-	-	0/11/31/31	0/1/1/1
2	NAG	B	702	1	-	0/6/23/26	0/1/1/1
2	NAG	B	705	1	-	0/6/23/26	0/1/1/1
4	HEM	B	706	1,7	-	0/6/54/54	0/0/8/8
5	IXP	B	707	-	-	0/38/77/77	0/8/8/8
2	NAG	C	701	1	-	0/6/23/26	0/1/1/1
2	NAG	C	704	1	-	0/6/23/26	0/1/1/1
4	HEM	C	705	1,7	-	0/6/54/54	0/0/8/8
5	IXP	C	706	-	-	0/38/77/77	0/8/8/8
2	NAG	D	701	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	704	1	-	0/6/23/26	0/1/1/1
4	HEM	D	705	1,7	-	0/6/54/54	0/0/8/8
6	BOG	D	706	-	-	0/11/31/31	0/1/1/1
5	IXP	D	707	-	-	0/38/77/77	0/8/8/8

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	707	IXP	CAZ-CAL	-10.19	1.39	1.52
5	A	706	IXP	CAZ-CAL	-10.18	1.39	1.52
5	D	707	IXP	CAZ-CAL	-10.18	1.39	1.52
5	A	706	IXP	CAK-CAX	-9.99	1.38	1.51
5	B	707	IXP	CAK-CAX	-9.95	1.38	1.51

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	IXP	CAJ-CAK-CAX	-6.93	93.07	102.78
5	A	706	IXP	CAV-OAW-CAX	-6.00	104.56	110.18
5	D	707	IXP	CAV-OAW-CAX	-5.97	104.59	110.18
5	B	707	IXP	CAV-OAW-CAX	-5.96	104.60	110.18
5	D	707	IXP	OAY-CAX-CAK	-5.86	122.42	129.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAG	2	0
4	A	705	HEM	2	0
5	A	706	IXP	7	0
6	B	701	BOG	4	0
2	B	702	NAG	1	0
4	B	706	HEM	2	0
5	B	707	IXP	13	0
2	C	701	NAG	2	0
4	C	705	HEM	2	0
5	C	706	IXP	7	0
2	D	701	NAG	2	0
4	D	705	HEM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	706	BOG	1	0
5	D	707	IXP	13	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, 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	552/587 (94%)	-0.06	25 (4%) 37 45	19, 32, 63, 86	0
1	B	551/587 (93%)	-0.07	24 (4%) 38 47	20, 36, 69, 97	0
1	C	552/587 (94%)	-0.11	27 (4%) 33 42	17, 28, 58, 88	0
1	D	551/587 (93%)	-0.24	16 (2%) 55 63	18, 29, 54, 82	0
All	All	2206/2348 (93%)	-0.12	92 (4%) 40 48	17, 31, 62, 97	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	6.7
1	B	74	PHE	6.6
1	B	81	LEU	5.5
1	A	81	LEU	5.4
1	B	105(A)	ILE	5.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	702	14/15	0.95	0.10	0.13	23,32,36,41	0
3	NAG	D	702	14/15	0.95	0.09	0.08	21,31,38,45	0
3	NAG	A	702	14/15	0.96	0.10	-0.02	23,37,43,45	0
3	NAG	B	703	14/15	0.94	0.09	-0.38	30,34,38,43	0
3	NAG	D	703	14/15	0.88	0.17	-	51,57,62,63	0
3	NAG	A	703	14/15	0.88	0.13	-	46,54,61,63	0
3	NAG	B	704	14/15	0.88	0.16	-	47,51,61,65	0
3	NAG	C	703	14/15	0.89	0.13	-	43,50,60,61	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BOG	B	701	20/20	0.85	0.17	1.73	42,49,55,55	0
2	NAG	D	704	14/15	0.91	0.22	1.53	39,50,54,59	0
2	NAG	B	705	14/15	0.88	0.21	0.98	53,58,63,66	0
5	IXP	D	707	66/66	0.82	0.21	0.87	25,35,78,83	34
4	HEM	A	705	43/43	0.96	0.12	0.80	22,27,52,64	0
4	HEM	C	705	43/43	0.96	0.13	0.73	17,22,44,55	0
5	IXP	B	707	66/66	0.88	0.17	0.50	30,32,48,60	41
4	HEM	D	705	43/43	0.95	0.11	0.25	19,25,45,52	0
2	NAG	C	704	14/15	0.91	0.10	0.03	35,44,49,55	0
2	NAG	A	704	14/15	0.89	0.10	-0.08	42,50,57,61	0
5	IXP	A	706	66/66	0.89	0.15	-0.24	30,37,62,71	34
4	HEM	B	706	43/43	0.96	0.11	-0.25	26,31,55,66	0
6	BOG	D	706	20/20	0.94	0.09	-0.27	29,39,54,54	0
5	IXP	C	706	66/66	0.88	0.14	-0.51	30,30,44,55	41
2	NAG	B	702	14/15	0.78	0.26	-	70,74,76,80	0
2	NAG	D	701	14/15	0.79	0.21	-	49,59,62,64	0
2	NAG	A	701	14/15	0.78	0.24	-	57,65,75,77	0
2	NAG	C	701	14/15	0.81	0.27	-	52,64,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.