

# wwPDB X-ray Structure Validation Summary Report (i)

Nov 30, 2022 - 12:34 am GMT

PDB ID	:	7YXD
Title	:	Crystal structure of WT AncGR2-LBD bound to dexame thas one and SHP
		coregulator fragment
Authors	:	Jimenez-Panizo, A.; Estebanez-Perpina, E.; Fuentes-Prior, P.
Deposited on	:	2022-02-15
Resolution	:	2.30 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

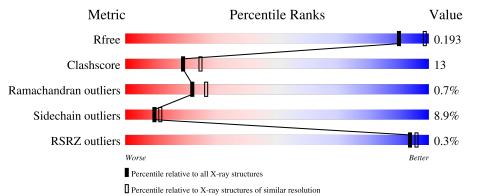
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.30 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	248	69%	25%	•••
1	D	248	71%	22%	
1	Н	248	69%	24%	••
1	L	248	70%	23%	•••
2	С	12	50%	42%	8%

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Mol	Chain		Quality of	chain		
2	F	12	58%	3:	3%	8%
2	J	12	8%	25%	17%	8%
2	Ν	12	50%	33%	8%	8%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8280 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	241	Total	С	Ν	N O S		0	1	0
	А	241	1958	1271	318	351	18	0		0
1	Л	240	Total	С	Ν	0	S	0	1	0
		240	1946	1261	317	350	18	0	1	0
1	Н	241	Total	С	Ν	0	S	0	0	0
	п	241	1956	1270	318	351	17	0	0	0
1	т	241	Total	С	Ν	0	S	0	1	0
		241	1957	1270	318	351	18	0		U

• Molecule 1 is a protein called Ancestral Glucocorticoid Receptor2.

There are 4 discrepancies between the modelled and reference sequences:

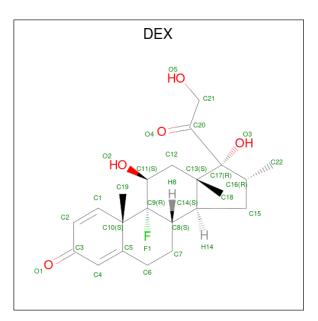
Chain	Residue	Modelled	Actual	Comment	Reference
А	529	PHE	-	expression tag	UNP A0A1X8XLE9
D	529	PHE	-	expression tag	UNP A0A1X8XLE9
Н	529	PHE	-	expression tag	UNP A0A1X8XLE9
L	529	PHE	-	expression tag	UNP A0A1X8XLE9

• Molecule 2 is a protein called SHP NR Box 1 Peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	11	Total C N O	0	0	0
2	U	11	84  56  14  14	0	0	0
2	F	11	Total C N O	0	0	0
	Г	11	84  56  14  14	0	0	0
2	J	12	Total C N O	0	0	0
	J	12	90 $59$ $15$ $16$	0	0	0
2	N	11	Total C N O	0	0	0
	1N		84 56 14 14	0	0	0

• Molecule 3 is DEXAMETHASONE (three-letter code: DEX) (formula:  $C_{22}H_{29}FO_5$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total         C         F         O           28         22         1         5	0	0
3	D	1	Total         C         F         O           28         22         1         5	0	0
3	Н	1	Total         C         F         O           28         22         1         5	0	0
3	L	1	Total         C         F         O           28         22         1         5	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	1	Total Na 1 1	0	0

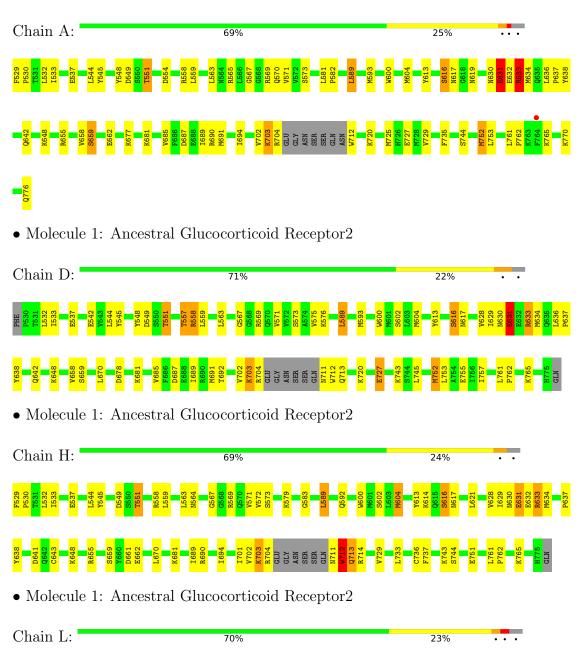
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	4	Total O 4 4	0	0
5	D	1	Total O 1 1	0	0
5	Н	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Ancestral Glucocorticoid Receptor2



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 $\bullet$  Molecule 2: SHP NR Box 1 Peptide

Chain C:	50%	42%		8%
R17 120 120 121 120 123 124 124 124 124 125 226 226 226 226 226 226 226 226 226 2				
• Molecule 2: SHI	P NR Box 1 Peptide			
Chain F:	58%	339	6	8%
R17 P18 A19 120 120 SER SER				
• Molecule 2: SHI	P NR Box 1 Peptide			
Chain J:	50%	25%	17%	8%
R17 120 120 121 121 125 125 125 827 826 828 528				
• Molecule 2: SHI	P NR Box 1 Peptide			
Chain N:	50%	33%	8%	8%
R17 120 121 121 123 123 124 124 126 825 826 827 827 827 827				



# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 31	Depositor	
Cell constants	107.60Å $107.60$ Å $135.64$ Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	76.81 - 2.30	Depositor	
Resolution (A)	76.81 - 2.30	EDS	
% Data completeness	94.4 (76.81-2.30)	Depositor	
(in resolution range)	94.4(76.81-2.30)	EDS	
R <sub>merge</sub>	(Not available)	Depositor	
$\frac{\mathbf{R}_{sym}}{< I/\sigma(I) > 1}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.41 (at 2.29 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.8.0267	Depositor	
D D	0.177 , $0.221$	Depositor	
$R, R_{free}$	0.149 , $0.193$	DCC	
$R_{free}$ test set	3768 reflections $(5.11%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	45.0	Xtriage	
Anisotropy	0.005	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS	
L-test for twinning <sup>2</sup>	$< L >=0.39, < L^2>=0.22$	Xtriage	
	0.450 for -h,-k,l		
Estimated twinning fraction	0.449 for h,-h-k,-l	Xtriage	
	0.449 for -k,-h,-l		
	0.265 for H, K, L		
Reported twinning fraction	0.240 for K, H, -L	Depositor	
Reported twinning fraction	0.237 for -K, -H, -L	Depositor	
	0.259 for -h,-k,l		
Outliers	0 of 73666 reflections	Xtriage	
$F_o, F_c$ correlation	0.97	EDS	
Total number of atoms	8280	wwPDB-VP	
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: DEX, NA

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	Boi	nd lengths	B	ond angles
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.52	0/2006	0.99	1/2707~(0.0%)
1	D	0.56	1/1993~(0.1%)	1.01	3/2689~(0.1%)
1	Н	0.53	0/1999	1.01	2/2698~(0.1%)
1	L	0.53	0/2005	1.04	6/2706~(0.2%)
2	С	0.73	0/85	0.98	0/115
2	F	0.84	0/85	1.02	0/115
2	J	0.77	0/91	1.12	0/123
2	Ν	0.65	0/85	1.18	0/115
All	All	0.54	1/8349~(0.0%)	1.01	12/11268~(0.1%)

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	А	0	2
1	D	0	1
1	Н	0	1
1	L	0	2
2	J	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	D	631	GLU	CD-OE2	7.50	1.33	1.25

The worst 5 of 12 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	L	681	LYS	CB-CA-C	6.60	123.61	110.40
1	А	633	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	L	615	GLN	CB-CA-C	6.42	123.25	110.40
1	D	692	THR	CA-CB-OG1	-6.16	96.06	109.00
1	L	732	LEU	CB-CG-CD1	-5.84	101.07	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	631	GLU	Peptide
1	А	712	TRP	Peptide
1	D	631	GLU	Peptide
1	Н	631	GLU	Peptide
2	J	27	SER	Peptide

### 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	А	1958	0	1991	50	0
1	D	1946	0	1981	55	0
1	Н	1956	0	1986	57	0
1	L	1957	0	1989	45	0
2	С	84	0	92	10	0
2	F	84	0	92	11	0
2	J	90	0	97	9	0
2	Ν	84	0	92	8	0
3	А	28	0	29	4	0
3	D	28	0	29	3	0
3	Н	28	0	29	5	0
3	L	28	0	29	3	0
4	Н	1	0	0	0	0
5	А	4	0	0	0	0
5	D	1	0	0	0	0
5	Н	2	0	0	0	0
5	L	1	0	0	0	0
All	All	8280	0	8436	218	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 13.

The worst 5 of 218 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:H:711:ASN:O	1:H:713:GLN:N	1.60	1.30
1:H:641:ASP:OD1	1:L:742:ASN:ND2	1.78	1.14
1:L:630:ASN:OD1	1:L:633:ARG:HG3	1.49	1.11
1:A:593:MET:HE1	2:C:22:TYR:HB2	1.51	0.90
1:H:600:TRP:O	1:H:604:MET:HG2	1.71	0.90

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	Perce	entiles
1	А	238/248~(96%)	228~(96%)	8(3%)	2(1%)	19	23
1	D	237/248~(96%)	228~(96%)	8~(3%)	1 (0%)	34	42
1	Н	237/248~(96%)	229~(97%)	6~(2%)	2(1%)	19	23
1	L	238/248~(96%)	228~(96%)	8~(3%)	2(1%)	19	23
2	С	9/12~(75%)	$8 \ (89\%)$	1 (11%)	0	100	100
2	F	9/12~(75%)	9 (100%)	0	0	100	100
2	J	10/12~(83%)	8~(80%)	2(20%)	0	100	100
2	Ν	9/12~(75%)	9 (100%)	0	0	100	100
All	All	987/1040~(95%)	947~(96%)	33~(3%)	7~(1%)	22	26

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type		
1	Η	712	TRP		
Continued on most mana					

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Mol	Chain	Res	Type
1	L	616	SER
1	D	703	LYS
1	Н	703	LYS
1	L	703	LYS

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	222/227~(98%)	205~(92%)	17 (8%)	13 16
1	D	221/227~(97%)	202~(91%)	19 (9%)	10 12
1	Н	221/227~(97%)	205~(93%)	16 (7%)	14 18
1	L	222/227~(98%)	198 (89%)	24 (11%)	6 7
2	С	9/10~(90%)	8 (89%)	1 (11%)	6 7
2	F	9/10~(90%)	9 (100%)	0	100 100
2	J	10/10~(100%)	6~(60%)	4 (40%)	0
2	Ν	9/10~(90%)	8 (89%)	1 (11%)	6 7
All	All	923/948~(97%)	841 (91%)	82 (9%)	9 11

 $5~{\rm of}~82$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	L	532	LEU
1	L	681	LYS
1	L	551	THR
1	L	615	GLN
1	L	727	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	А	644	GLN



#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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).

Mal	Mol Type	Chain	Chain	Chain	Res	Res Link	Bo	Bond lengths			Bond angles		
Mol Type	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2				
3	DEX	L	1001	-	31,31,31	0.77	0	$52,\!53,\!53$	1.98	17 (32%)			
3	DEX	D	1001	-	31,31,31	0.80	0	52,53,53	2.22	15 (28%)			
3	DEX	Н	1001	-	31,31,31	0.63	0	52,53,53	2.50	19 (36%)			
3	DEX	А	1001	-	31,31,31	0.60	0	52,53,53	2.27	20 (38%)			

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	DEX	L	1001	-	-	1/8/84/84	0/4/4/4
3	DEX	D	1001	-	-	2/8/84/84	0/4/4/4
3	DEX	Н	1001	-	-	1/8/84/84	0/4/4/4
3	DEX	A	1001	-	-	2/8/84/84	0/4/4/4



There are no bond length outliers.

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	1001	DEX	F1-C9-C8	-6.74	99.89	105.95
3	Н	1001	DEX	O2-C11-C9	-6.58	99.35	109.08
3	А	1001	DEX	C19-C10-C9	6.37	118.11	113.55
3	А	1001	DEX	C13-C17-C20	-6.26	106.25	112.89
3	Н	1001	DEX	C6-C5-C10	6.02	119.32	115.61

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1001	DEX	C17-C20-C21-O5
3	D	1001	DEX	O4-C20-C21-O5
3	А	1001	DEX	C17-C20-C21-O5
3	L	1001	DEX	C17-C20-C21-O5
3	А	1001	DEX	O4-C20-C21-O5

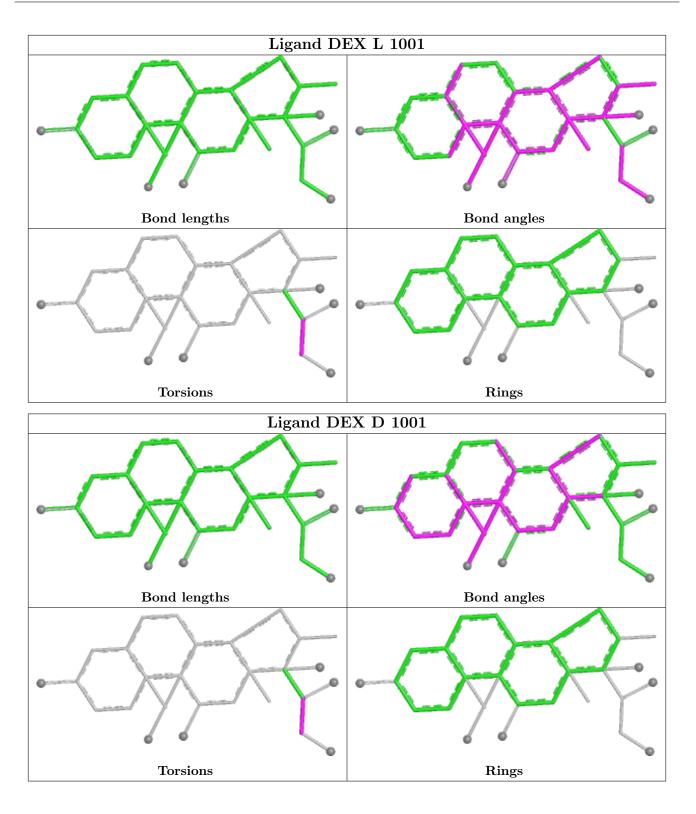
There are no ring outliers.

4 monomers are involved in 15 short contacts:

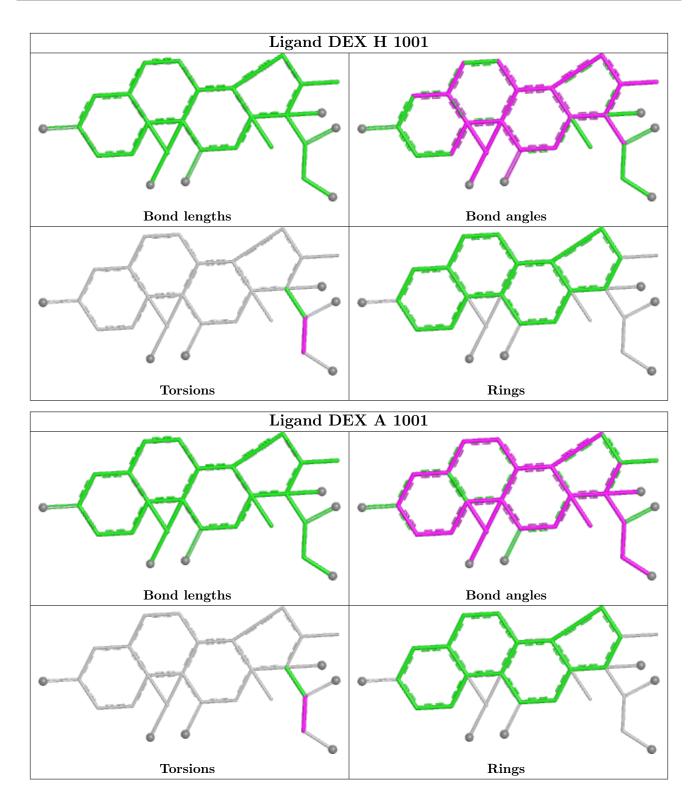
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1001	DEX	3	0
3	D	1001	DEX	3	0
3	Н	1001	DEX	5	0
3	А	1001	DEX	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









# 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,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	241/248~(97%)	-0.21	1 (0%) 92 95	22,  46,  78,  154	0
1	D	240/248~(96%)	-0.23	0 100 100	24, 47, 71, 96	0
1	Н	241/248~(97%)	-0.27	0 100 100	25,  48,  72,  100	0
1	L	241/248~(97%)	-0.25	1 (0%) 92 95	18, 49, 80, 104	0
2	С	11/12~(91%)	-0.30	0 100 100	39, 51, 58, 66	0
2	F	11/12~(91%)	-0.27	0 100 100	31,  44,  61,  63	0
2	J	12/12~(100%)	-0.15	1 (8%) 11 15	21, 54, 70, 98	0
2	Ν	$11/12 \ (91\%)$	-0.19	0 100 100	33, 51, 67, 73	0
All	All	1008/1040~(96%)	-0.24	3 (0%) 94 96	18, 48, 76, 154	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	764	PHE	6.8
2	J	22	TYR	2.5
1	L	764	PHE	2.1

### 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)

There are no monosaccharides in this entry.

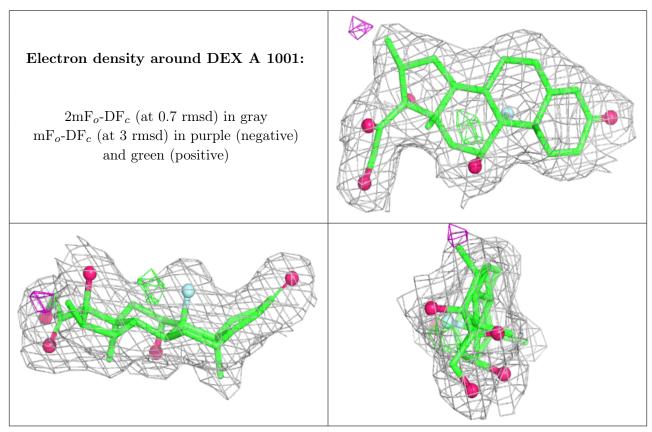


### 6.4 Ligands (i)

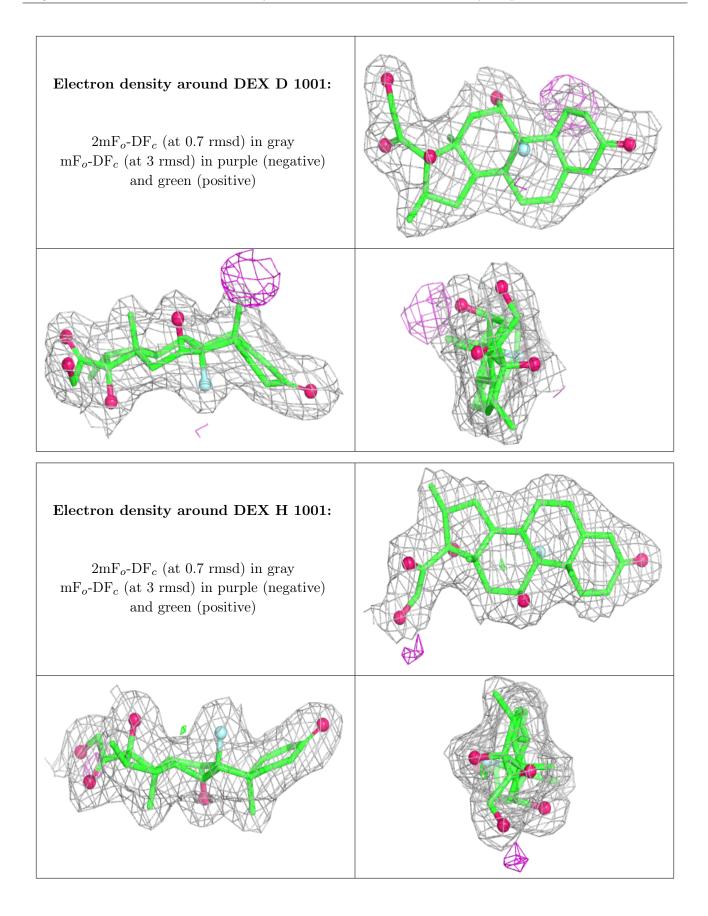
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	DEX	А	1001	28/28	0.99	0.11	21,26,31,32	0
3	DEX	D	1001	28/28	0.99	0.11	21,29,37,40	0
3	DEX	Н	1001	28/28	0.99	0.12	19,25,35,41	0
3	DEX	L	1001	28/28	0.99	0.12	19,26,34,45	0
4	NA	Н	1002	1/1	1.00	0.11	23,23,23,23	0

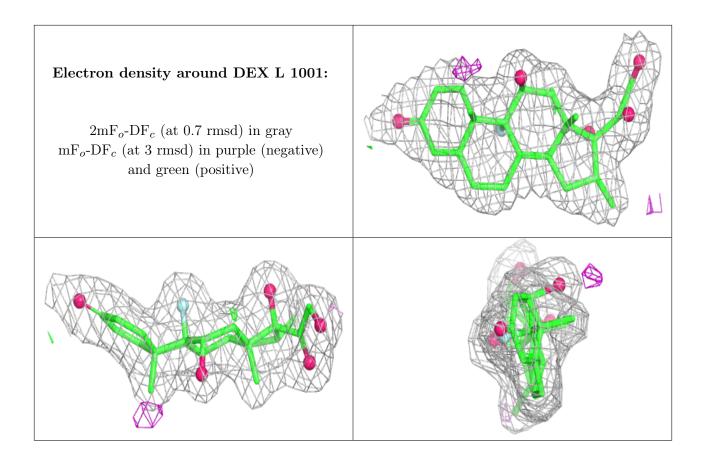
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











### 6.5 Other polymers (i)

There are no such residues in this entry.

