



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:08 AM UTC

PDB ID : 7YXN / pdb_00007yxn
Title : Crystal structure of WT AncGR2-LBD bound to dexamethasone and SHP coregulator fragment
Authors : Jimenez-Panizo, A.; Estebanez-Perpina, E.; Fuentes-Prior, P.
Deposited on : 2022-02-16
Resolution : 2.46 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

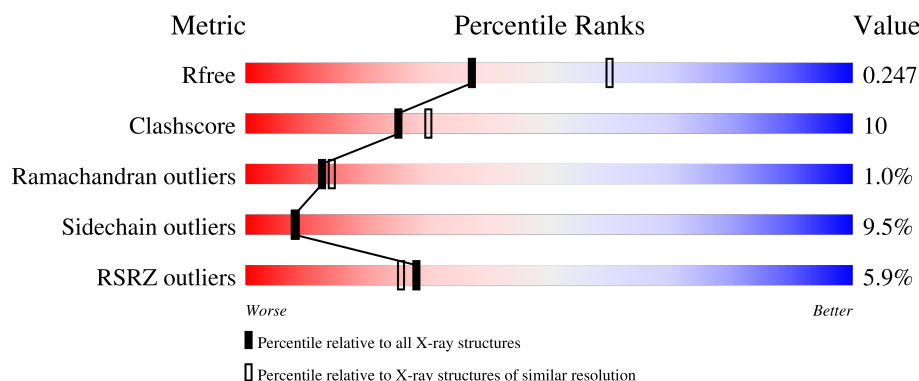
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 $\leq 5\%$. 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	250	6% 73% 21% ...
1	C	250	6% 71% 23% ..
2	R	11	18% 82% 18%
2	S	11	64% 27% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4190 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 Ancestral Glucocorticoid Receptor2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	2	0
			1971	1277	320	356	18			
1	C	244	Total	C	N	O	S	0	0	0
			1978	1282	322	357	17			

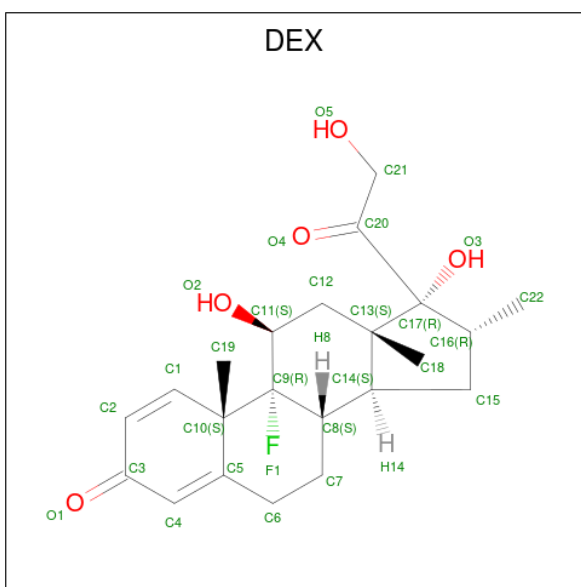
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	GLY	-	expression tag	UNP A0A1X8XLE9
A	528	GLU	-	expression tag	UNP A0A1X8XLE9
A	529	PHE	-	expression tag	UNP A0A1X8XLE9
C	527	GLY	-	expression tag	UNP A0A1X8XLE9
C	528	GLU	-	expression tag	UNP A0A1X8XLE9
C	529	PHE	-	expression tag	UNP A0A1X8XLE9

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

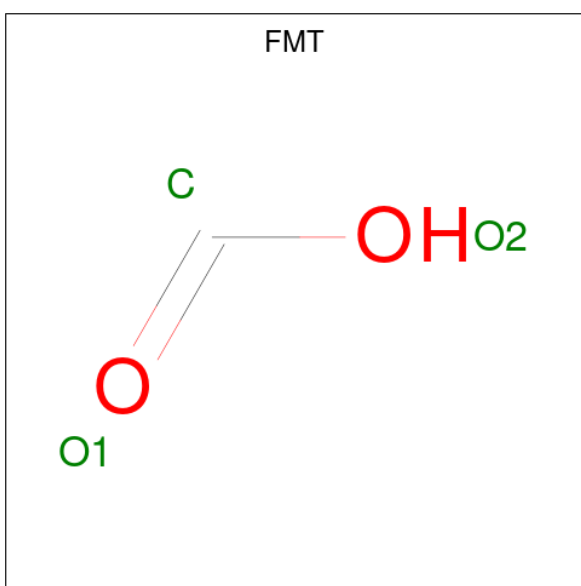
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	R	11	Total	C	N	O	0	0	0
			84	56	14	14			
2	S	11	Total	C	N	O	0	0	0
			84	56	14	14			

- Molecule 3 is DEXAMETHASONE (CCD ID: DEX) (formula: C₂₂H₂₉FO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			28	22	1	5		
3	C	1	Total	C	F	O	0	0
			28	22	1	5		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		

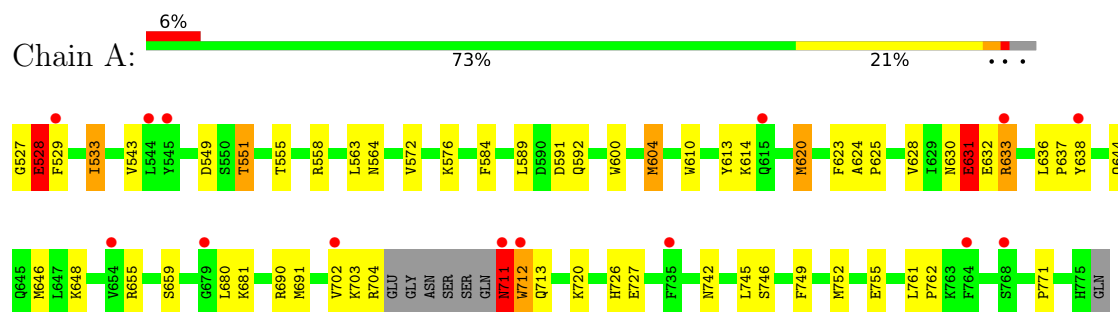
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	C	1	Total	O	0	0
			1	1		
5	S	1	Total	O	0	0
			1	1		

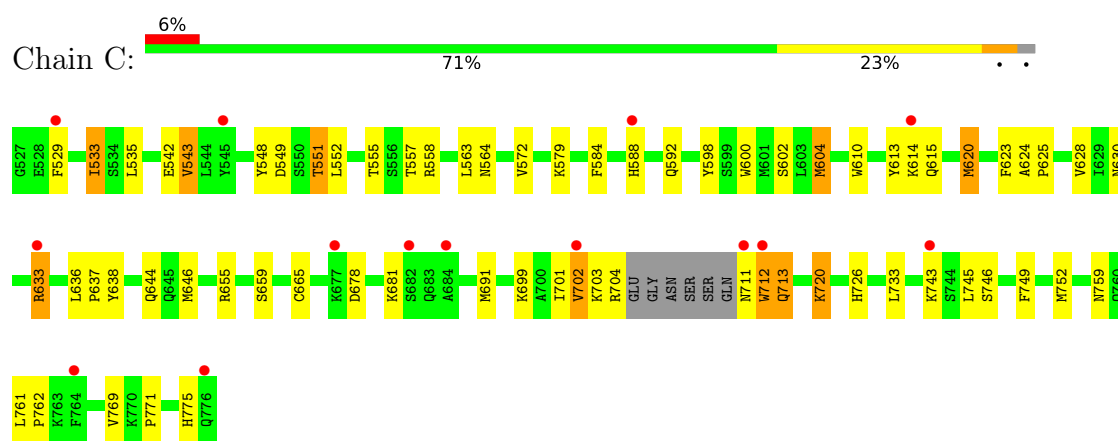
3 Residue-property plots [i](#)

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.

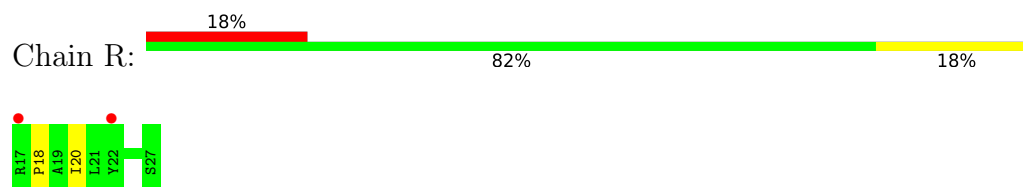
• Molecule 1: Ancestral Glucocorticoid Receptor2



• Molecule 1: Ancestral Glucocorticoid Receptor2



• Molecule 2: SHP NR Box 1 Peptide



• Molecule 2: SHP NR Box 1 Peptide



R17	P18	L24	L25	S26	S27
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	109.48Å 109.48Å 137.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	94.81 – 2.46 94.81 – 2.46	Depositor EDS
% Data completeness (in resolution range)	96.5 (94.81-2.46) 96.5 (94.81-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.247 0.216 , 0.247	Depositor DCC
R_{free} test set	1692 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.075 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4190	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.60	0/2024	1.27	11/2731 (0.4%)
1	C	0.61	0/2021	1.20	4/2727 (0.1%)
2	R	0.75	0/85	1.19	0/115
2	S	0.63	0/85	1.06	0/115
All	All	0.61	0/4215	1.23	15/5688 (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	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	712	TRP	N-CA-C	-11.65	99.55	113.88
1	C	557	THR	CA-CB-OG1	-6.88	99.28	109.60
1	A	633	ARG	CG-CD-NE	-6.70	97.27	112.00
1	A	711	ASN	CB-CA-C	6.60	122.64	110.10
1	A	631	GLU	CB-CA-C	5.97	120.71	111.28
1	A	633	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	712	TRP	CA-C-N	5.87	128.62	120.29
1	A	712	TRP	C-N-CA	5.87	128.62	120.29
1	A	648	LYS	CB-CA-C	5.64	119.84	110.81
1	A	529	PHE	CA-CB-CG	5.39	119.19	113.80
1	C	701	ILE	CA-C-N	5.37	127.41	120.70
1	C	701	ILE	C-N-CA	5.37	127.41	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	615	GLN	CB-CA-C	5.19	120.28	109.95
1	A	712	TRP	N-CA-CB	-5.10	103.81	110.59
1	A	713	GLN	N-CA-C	-5.07	105.83	111.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	631	GLU	Peptide
1	A	632	GLU	Peptide
1	A	711	ASN	Mainchain

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	1971	0	1999	38	0
1	C	1978	0	2005	44	0
2	R	84	0	92	1	0
2	S	84	0	92	2	0
3	A	28	0	29	1	0
3	C	28	0	29	1	0
4	A	6	0	2	0	0
4	C	6	0	2	0	0
5	A	3	0	0	0	0
5	C	1	0	0	0	0
5	S	1	0	0	0	0
All	All	4190	0	4250	82	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 10.

All (82) 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:C:726:HIS:ND1	1:C:771:PRO:HB3	1.85	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:HIS:ND1	1:A:771:PRO:HB3	1.87	0.89
1:A:620:MET:HE3	1:A:628:VAL:CG1	2.11	0.80
1:A:527:GLY:O	1:A:528:GLU:HB2	1.84	0.77
1:C:712:TRP:C	1:C:712:TRP:CD1	2.62	0.76
1:A:620:MET:HE3	1:A:628:VAL:HG11	1.68	0.76
1:C:620:MET:HE2	1:C:628:VAL:CG1	2.17	0.73
1:C:572:VAL:HG22	1:C:752:MET:HE2	1.69	0.72
1:A:659:SER:HB3	1:A:704:ARG:HD2	1.72	0.71
1:A:572:VAL:HG22	1:A:752:MET:HE2	1.72	0.71
1:C:699:LYS:O	1:C:702:VAL:HB	1.91	0.70
1:A:630:ASN:OD1	1:A:633:ARG:HG2	1.93	0.69
1:C:604:MET:HE2	1:C:604:MET:HA	1.76	0.67
1:C:548:TYR:HE2	1:C:633:ARG:NH2	1.93	0.66
1:A:620:MET:CE	1:A:628:VAL:HG11	2.25	0.66
1:A:591:ASP:OD2	1:A:680:LEU:HB3	1.99	0.63
1:C:588:HIS:ND1	1:C:681:LYS:HD2	2.15	0.62
1:A:702:VAL:C	1:A:704:ARG:H	2.09	0.60
1:A:604:MET:HA	1:A:604:MET:CE	2.32	0.60
1:C:564:ASN:ND2	1:C:749:PHE:CE1	2.71	0.59
1:A:527:GLY:O	1:A:528:GLU:CB	2.50	0.59
1:C:543:VAL:CG1	1:C:543:VAL:O	2.50	0.59
1:C:579:LYS:HE3	2:S:25:LEU:HA	1.82	0.59
1:C:600:TRP:O	1:C:604:MET:HG2	2.04	0.58
1:A:755:GLU:OE2	2:R:20:ILE:HG13	2.04	0.58
1:C:548:TYR:HE2	1:C:633:ARG:HH21	1.50	0.58
1:C:637:PRO:O	1:C:638:TYR:HB2	2.02	0.58
1:A:604:MET:HA	1:A:604:MET:HE2	1.85	0.57
1:A:624:ALA:HB1	1:A:625:PRO:CD	2.34	0.57
1:A:572:VAL:CG2	1:A:752:MET:HE2	2.35	0.56
1:C:702:VAL:C	1:C:704:ARG:H	2.14	0.56
1:C:620:MET:HE2	1:C:628:VAL:HG12	1.88	0.55
1:C:659:SER:HB3	1:C:704:ARG:HD2	1.89	0.55
1:A:610:TRP:CZ2	1:A:614:LYS:HE2	2.42	0.55
1:C:624:ALA:HB1	1:C:625:PRO:CD	2.37	0.54
1:A:646:MET:HE2	3:A:1001:DEX:H222	1.89	0.54
1:C:646:MET:HE2	3:C:1001:DEX:H222	1.89	0.54
1:C:655:ARG:HG2	1:C:655:ARG:HH11	1.73	0.53
1:A:655:ARG:HH11	1:A:655:ARG:HG2	1.74	0.53
1:A:600:TRP:O	1:A:604:MET:HG2	2.09	0.51
1:A:702:VAL:O	1:A:704:ARG:N	2.43	0.51
1:A:633:ARG:HB2	1:A:636:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:PRO:O	1:A:638:TYR:HB2	2.11	0.50
1:C:620:MET:HE2	1:C:628:VAL:HG11	1.92	0.50
1:C:584:PHE:CE2	1:C:592:GLN:HG2	2.46	0.50
1:A:584:PHE:CE2	1:A:592:GLN:HG2	2.47	0.50
1:A:702:VAL:C	1:A:704:ARG:N	2.70	0.49
1:C:548:TYR:CE2	1:C:633:ARG:NH2	2.76	0.49
1:A:620:MET:HE3	1:A:628:VAL:HG13	1.92	0.49
1:C:702:VAL:O	1:C:704:ARG:N	2.45	0.48
1:A:563:LEU:HD22	1:A:623:PHE:CD1	2.49	0.48
1:C:563:LEU:HD22	1:C:623:PHE:CD1	2.47	0.48
1:C:745:LEU:HD12	1:C:745:LEU:HA	1.73	0.48
1:A:630:ASN:OD1	1:A:630:ASN:C	2.56	0.47
1:C:702:VAL:C	1:C:704:ARG:N	2.70	0.47
1:C:633:ARG:HA	1:C:636:LEU:HD13	1.96	0.47
1:A:761:LEU:HB3	1:A:762:PRO:HD3	1.97	0.47
1:C:543:VAL:O	1:C:543:VAL:HG13	2.15	0.46
1:C:761:LEU:HB3	1:C:762:PRO:HD3	1.98	0.46
1:C:604:MET:HA	1:C:604:MET:CE	2.44	0.45
1:C:720:LYS:HG2	1:C:775:HIS:HD2	1.82	0.45
1:A:726:HIS:CE1	1:A:771:PRO:HB3	2.49	0.45
1:A:610:TRP:O	1:A:613:TYR:HB3	2.18	0.44
1:C:610:TRP:O	1:C:613:TYR:HB3	2.18	0.44
1:C:620:MET:CE	1:C:628:VAL:HG11	2.47	0.44
1:C:630:ASN:OD1	1:C:633:ARG:HG3	2.18	0.44
1:A:564:ASN:ND2	1:A:749:PHE:CE1	2.86	0.44
1:A:745:LEU:HD12	1:A:745:LEU:HA	1.71	0.43
1:C:549:ASP:C	1:C:551:THR:H	2.25	0.43
1:C:759:ASN:ND2	2:S:18:PRO:HD3	2.33	0.43
1:A:690:ARG:HH11	1:A:690:ARG:HD3	1.62	0.43
1:C:620:MET:CE	1:C:628:VAL:CG1	2.94	0.42
1:A:528:GLU:OE2	1:A:528:GLU:HA	2.18	0.42
1:C:549:ASP:HB3	1:C:552:LEU:HD12	2.02	0.42
1:C:598:TYR:CE1	1:C:769:VAL:HG22	2.55	0.41
1:A:742:ASN:OD1	1:A:745:LEU:HB2	2.19	0.41
1:A:533:ILE:HD12	1:A:533:ILE:HA	1.58	0.41
1:C:711:ASN:C	1:C:713:GLN:N	2.75	0.41
1:C:533:ILE:HD11	1:C:665:CYS:SG	2.61	0.41
1:A:549:ASP:C	1:A:551:THR:H	2.30	0.40
1:C:588:HIS:CE1	1:C:681:LYS:HD2	2.56	0.40
1:C:533:ILE:HD12	1:C:533:ILE:HA	1.95	0.40

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	241/250 (96%)	224 (93%)	15 (6%)	2 (1%)	16	20
1	C	240/250 (96%)	225 (94%)	14 (6%)	1 (0%)	30	37
2	R	9/11 (82%)	8 (89%)	0	1 (11%)	0	0
2	S	9/11 (82%)	7 (78%)	1 (11%)	1 (11%)	0	0
All	All	499/522 (96%)	464 (93%)	30 (6%)	5 (1%)	12	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	GLU
1	A	703	LYS
1	C	703	LYS
2	S	18	PRO
2	R	18	PRO

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	224/228 (98%)	205 (92%)	19 (8%)	10	11
1	C	223/228 (98%)	200 (90%)	23 (10%)	7	6
2	R	9/9 (100%)	9 (100%)	0	100	100
2	S	9/9 (100%)	7 (78%)	2 (22%)	1	0
All	All	465/474 (98%)	421 (90%)	44 (10%)	8	8

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	GLU
1	A	533	ILE
1	A	543	VAL
1	A	551	THR
1	A	555	THR
1	A	558	ARG
1	A	576	LYS
1	A	589	LEU
1	A	604	MET
1	A	620	MET
1	A	631	GLU
1	A	644	GLN
1	A	681	LYS
1	A	691	MET
1	A	711	ASN
1	A	712	TRP
1	A	720	LYS
1	A	727	GLU
1	A	746	SER
1	C	529	PHE
1	C	533	ILE
1	C	535	LEU
1	C	542	GLU
1	C	543	VAL
1	C	551	THR
1	C	555	THR
1	C	558	ARG
1	C	602	SER
1	C	604	MET
1	C	614	LYS
1	C	620	MET
1	C	633	ARG
1	C	644	GLN
1	C	678	ASP
1	C	691	MET
1	C	702	VAL
1	C	712	TRP
1	C	713	GLN
1	C	720	LYS
1	C	733	LEU
1	C	743	LYS
1	C	746	SER

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Mol	Chain	Res	Type
2	S	24	LEU
2	S	27	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	711	ASN
1	C	592	GLN
1	C	775	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	FMT	A	1002	-	2,2,2	0.12	0	1,1,1	0.29	0
3	DEX	C	1001	-	31,31,31	0.52	0	53,53,53	1.08	3 (5%)
3	DEX	A	1001	-	31,31,31	0.64	1 (3%)	53,53,53	1.01	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	C	1003	-	2,2,2	0.23	0	1,1,1	0.32	0
4	FMT	C	1002	-	2,2,2	0.29	0	1,1,1	0.17	0
4	FMT	A	1003	-	2,2,2	0.35	0	1,1,1	0.18	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	DEX	C	1001	-	-	0/8/84/84	0/4/4/4
3	DEX	A	1001	-	-	0/8/84/84	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	DEX	C10-C9	-2.14	1.55	1.57

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	DEX	C18-C13-C12	2.99	115.21	111.08
3	C	1001	DEX	C13-C17-C20	-2.98	108.97	112.86
3	C	1001	DEX	C6-C5-C10	2.67	117.47	115.70
3	A	1001	DEX	C12-C13-C17	-2.35	113.58	115.65
3	C	1001	DEX	C15-C14-C13	-2.26	101.64	103.98
3	A	1001	DEX	C9-C10-C1	-2.03	107.48	109.98

There are no chirality outliers.

There are no torsion outliers.

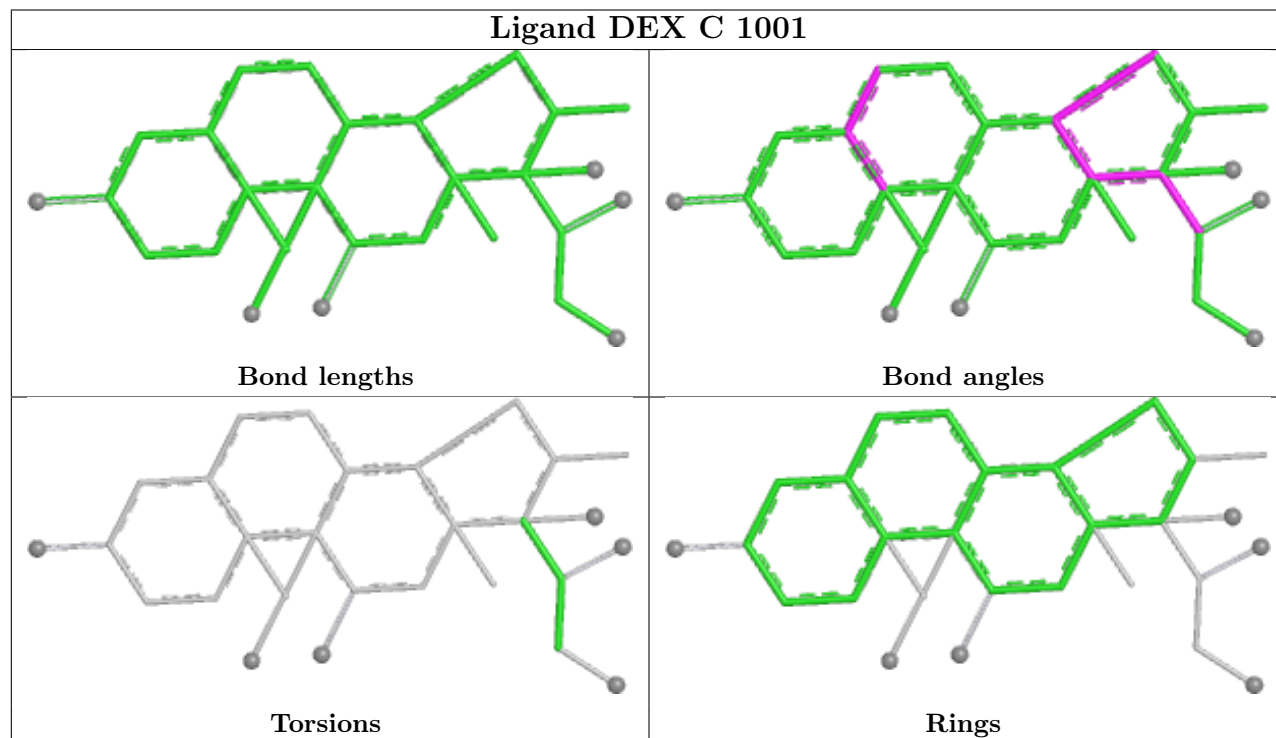
There are no ring outliers.

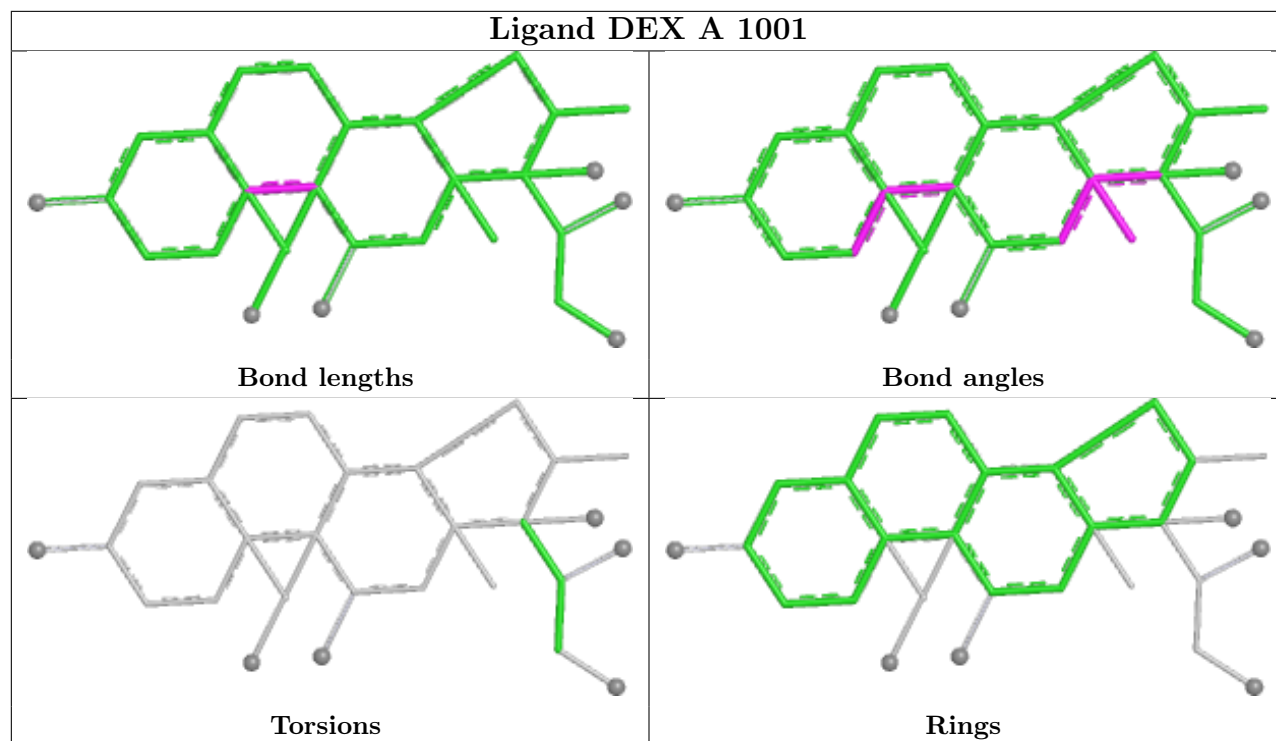
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	DEX	1	0
3	A	1001	DEX	1	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 than 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	243/250 (97%)	0.44	14 (5%)	29 26	35, 63, 104, 149	2 (0%)
1	C	244/250 (97%)	0.45	14 (5%)	29 26	33, 65, 106, 152	0
2	R	11/11 (100%)	1.22	2 (18%)	3 3	52, 73, 95, 123	0
2	S	11/11 (100%)	1.01	0	100 100	57, 72, 93, 121	0
All	All	509/522 (97%)	0.48	30 (5%)	28 25	33, 64, 106, 152	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	764	PHE	4.5
1	A	712	TRP	4.2
1	A	711	ASN	4.2
1	A	545	TYR	4.2
1	A	529	PHE	4.1
1	C	712	TRP	3.8
1	A	764	PHE	3.3
1	C	684	ALA	3.3
1	C	711	ASN	3.1
1	A	638	TYR	2.9
1	C	529	PHE	2.9
1	A	702	VAL	2.9
1	A	654	VAL	2.8
1	A	768	SER	2.6
2	R	22	TYR	2.6
1	C	545	TYR	2.5
1	A	544	LEU	2.4
1	C	776	GLN	2.4
1	C	682	SER	2.4
1	C	588	HIS	2.3
2	R	17	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	735	PHE	2.2
1	C	702	VAL	2.2
1	A	615	GLN	2.2
1	C	743	LYS	2.1
1	A	679	GLY	2.1
1	C	633	ARG	2.1
1	C	677	LYS	2.1
1	C	614	LYS	2.0
1	A	633	ARG	2.0

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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

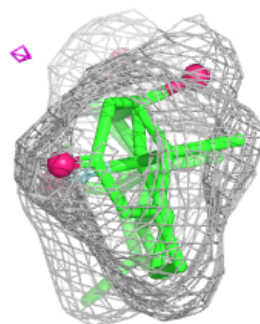
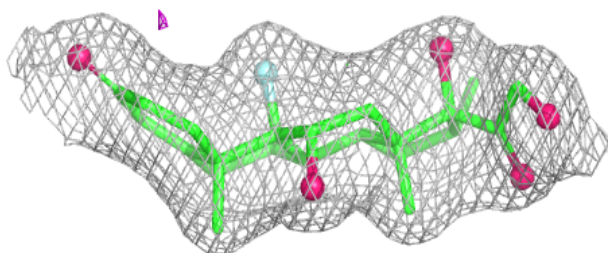
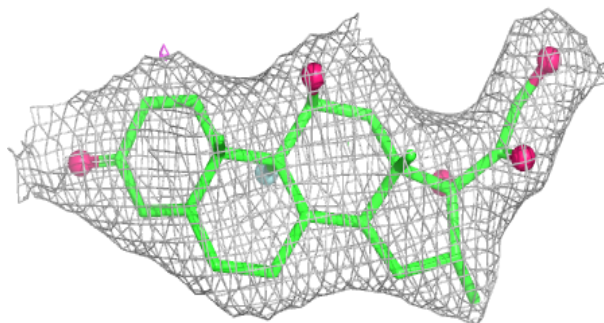
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	A	1003	3/3	0.85	0.20	77,77,79,87	0
4	FMT	C	1002	3/3	0.85	0.21	83,83,84,86	0
4	FMT	C	1003	3/3	0.88	0.17	66,66,69,70	0
4	FMT	A	1002	3/3	0.89	0.11	76,76,77,83	0
3	DEX	A	1001	28/28	0.96	0.07	30,41,46,51	0
3	DEX	C	1001	28/28	0.97	0.06	31,36,47,55	0

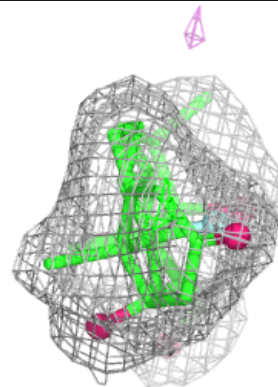
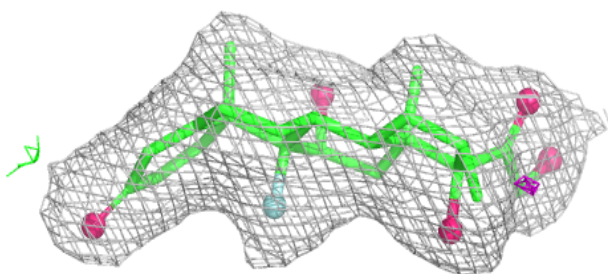
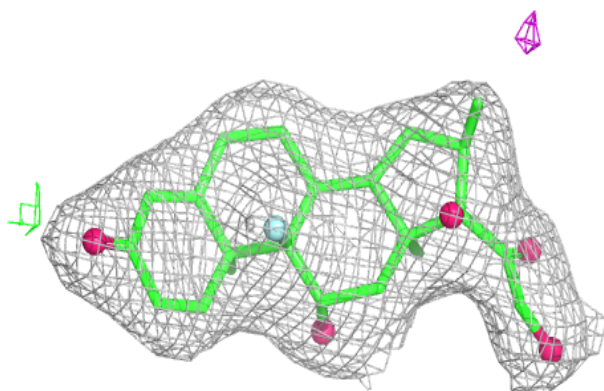
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DEX A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DEX C 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.