wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2023 – 05:16 PM EDT

PDB ID	:	1P93
Title	:	CRYSTAL STRUCTURE OF THE AGONIST FORM OF GLUCOCORTICOID RECEPTOR
Authors	:	Kauppi, B.; Jakob, C.; Farnegardh, M.; Yang, J.; Ahola, H.; Alarcon, M.; Calles, K.; Engstrom, O.; Harlan, J.; Muchmore, S.; Ramqvist, A.-K.; Thorell, S.; Ohman, L.; Greer, J.; Gustafsson, J.-A.; Carlstedt-Duke, J.; Carlquist, M.
Deposited on	:	2003-05-09
Resolution	:	2.70 Å(reported)

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

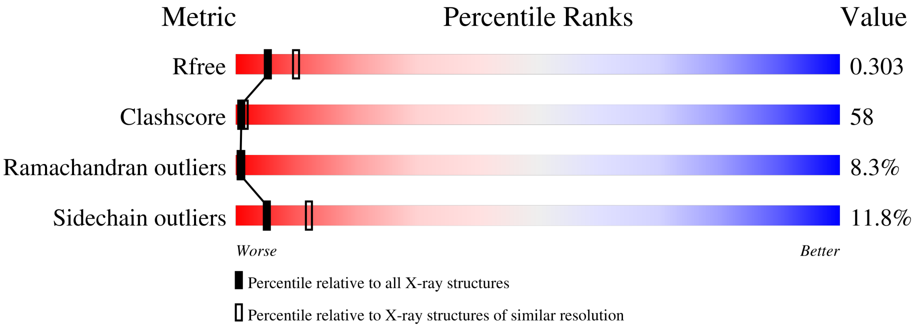
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

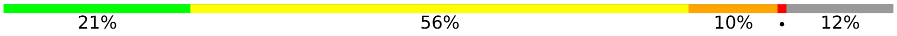
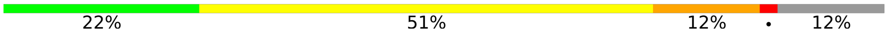
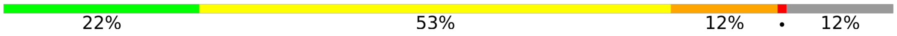
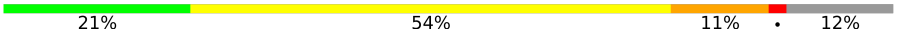
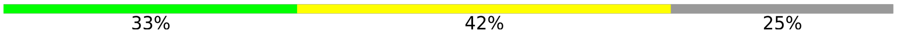
The reported resolution of this entry is 2.70 Å.

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Mol	**Chain**	**Length**	**Quality of chain**
1	A	280	 21% 56% 10% • 12%
1	B	280	 22% 51% 12% • 12%
1	C	280	 22% 53% 12% • 12%
1	D	280	 21% 54% 11% • 12%
2	E	12	 58% 17% 25%
2	F	12	 33% 42% 25%
2	G	12	 58% 17% 25%

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Mol	**Chain**	**Length**	**Quality of chain**
2	H	12	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8331 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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	2014	1299	331	367	17	0	0	0
1	B	245	1997	1288	328	364	17	0	0	0
1	C	247	2014	1299	331	367	17	0	0	0
1	D	247	2014	1299	331	367	17	0	0	0

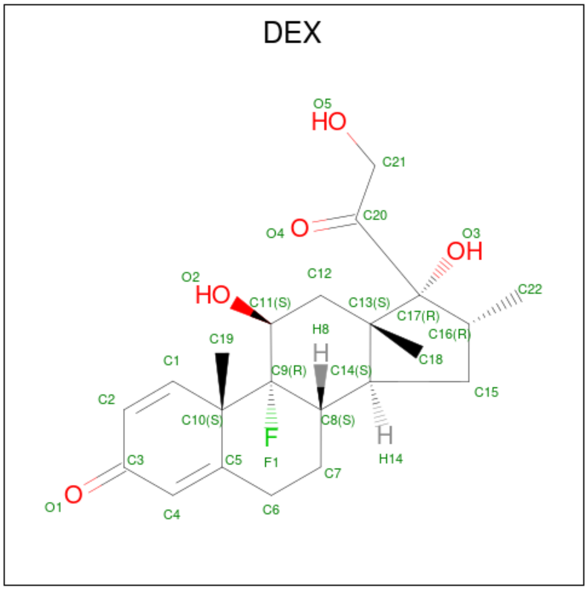
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	GLY	-	cloning artifact	UNP P04150
A	499	SER	-	cloning artifact	UNP P04150
A	517	ASP	ASN	engineered mutation	UNP P04150
A	602	SER	PHE	engineered mutation	UNP P04150
A	638	ASP	CYS	engineered mutation	UNP P04150
B	498	GLY	-	cloning artifact	UNP P04150
B	499	SER	-	cloning artifact	UNP P04150
B	517	ASP	ASN	engineered mutation	UNP P04150
B	602	SER	PHE	engineered mutation	UNP P04150
B	638	ASP	CYS	engineered mutation	UNP P04150
C	498	GLY	-	cloning artifact	UNP P04150
C	499	SER	-	cloning artifact	UNP P04150
C	517	ASP	ASN	engineered mutation	UNP P04150
C	602	SER	PHE	engineered mutation	UNP P04150
C	638	ASP	CYS	engineered mutation	UNP P04150
D	498	GLY	-	cloning artifact	UNP P04150
D	499	SER	-	cloning artifact	UNP P04150
D	517	ASP	ASN	engineered mutation	UNP P04150
D	602	SER	PHE	engineered mutation	UNP P04150
D	638	ASP	CYS	engineered mutation	UNP P04150

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	9	45	27	9	9	0	0	0
2	F	9	45	27	9	9	0	0	0
2	G	9	45	27	9	9	0	0	0
2	H	9	45	27	9	9	0	0	0

- Molecule 3 is DEXAMETHASONE (three-letter code: DEX) (formula: $C_{22}H_{29}FO_5$).

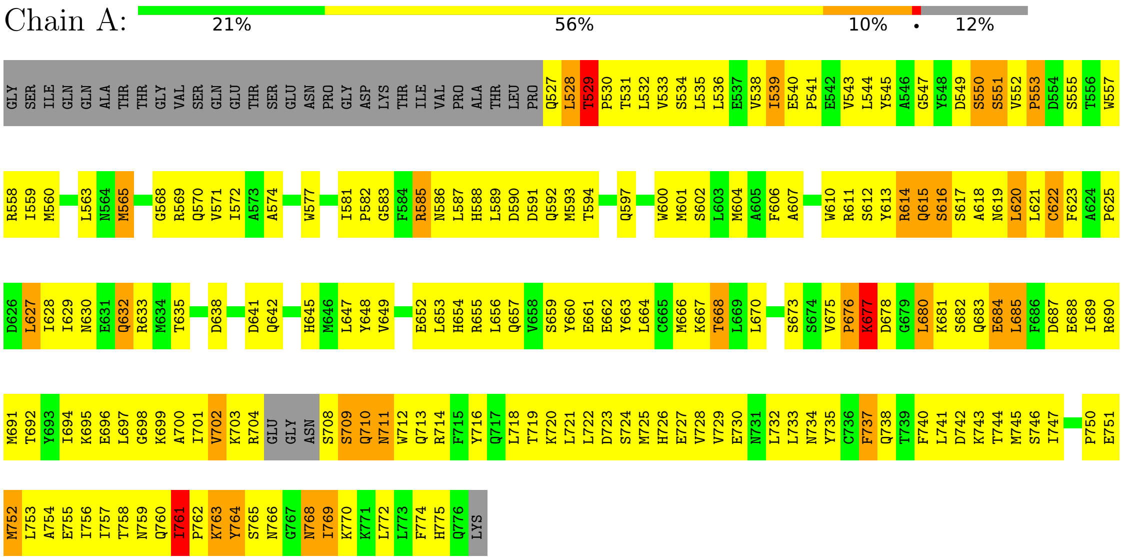


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
3	A	1	28	22	1	5	0	0
3	B	1	28	22	1	5	0	0
3	C	1	28	22	1	5	0	0
3	D	1	28	22	1	5	0	0

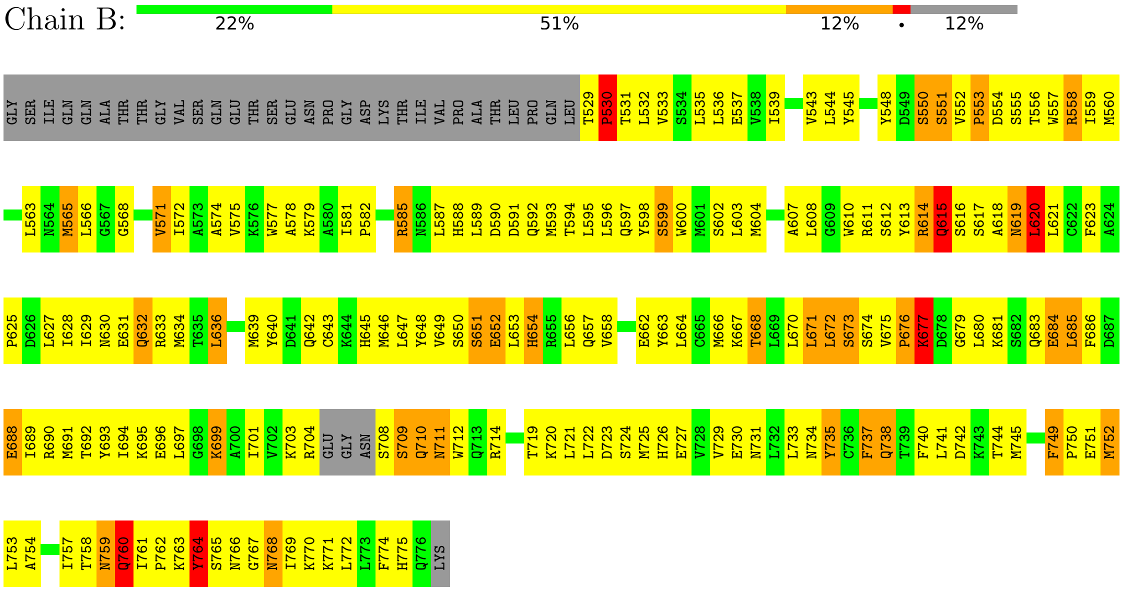
3 Residue-property plots

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. 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. 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.

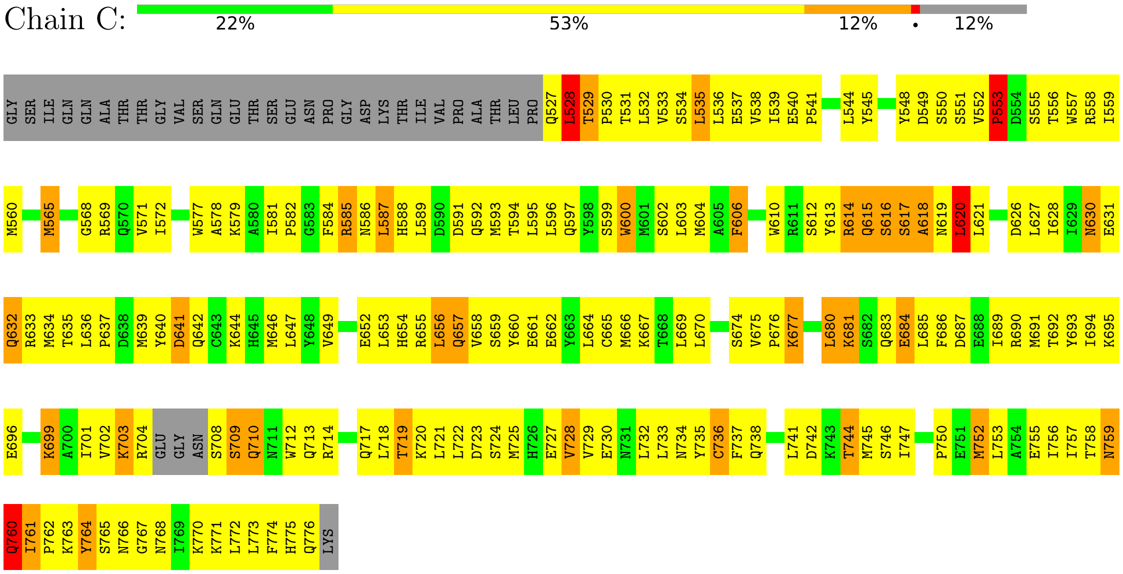
- Molecule 1: Glucocorticoid receptor



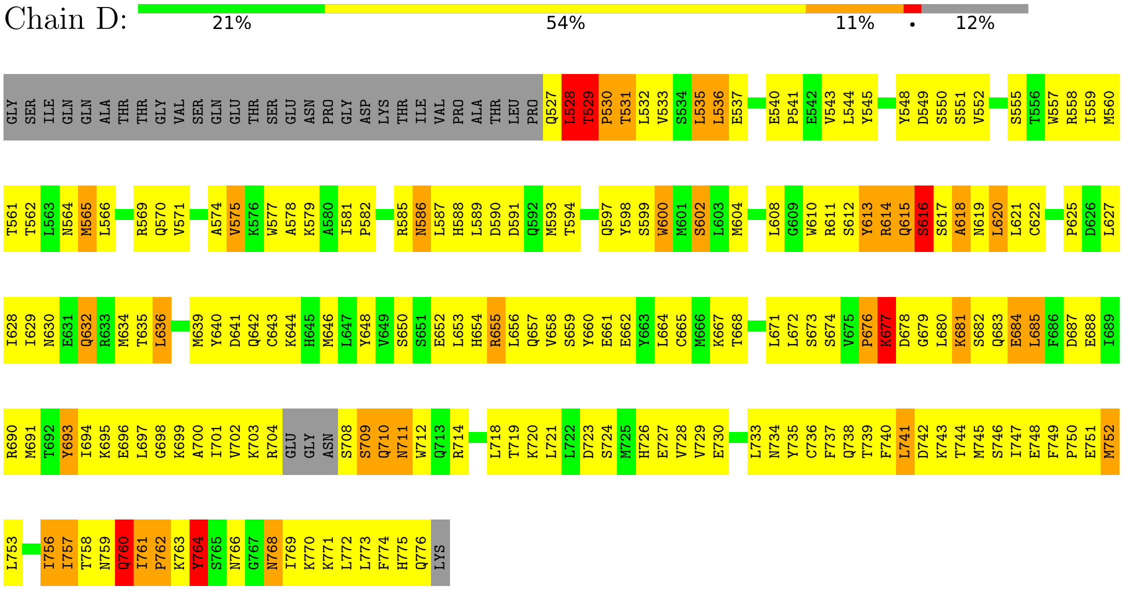
- Molecule 1: Glucocorticoid receptor



- Molecule 1: Glucocorticoid receptor

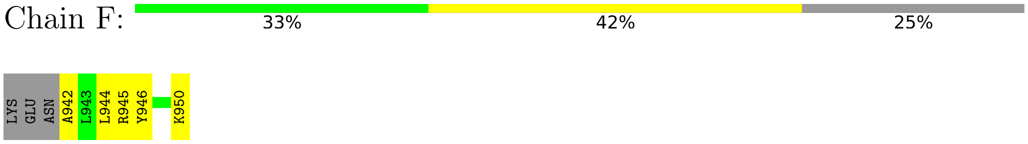


• Molecule 1: Glucocorticoid receptor



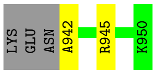
• Molecule 2: Nuclear receptor coactivator 2

• Molecule 2: Nuclear receptor coactivator 2



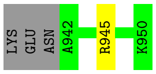
- Molecule 2: Nuclear receptor coactivator 2

Chain G:



- Molecule 2: Nuclear receptor coactivator 2

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	127.40Å 127.40Å 91.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.17 – 2.70 55.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.17-2.70) 99.9 (55.17-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.69Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.345 , 0.363 0.301 , 0.303	Depositor DCC
R_{free} test set	2310 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	74.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.129 for -h,-k,l 0.338 for h,-h-k,-l 0.126 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8331	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.47	0/2057	0.72	0/2782
1	B	0.50	0/2040	0.72	0/2759
1	C	0.48	0/2057	0.73	0/2782
1	D	0.52	0/2057	0.72	1/2782 (0.0%)
2	E	0.55	0/44	0.55	0/60
2	F	0.53	0/44	0.55	0/60
2	G	0.49	0/44	0.76	0/60
2	H	0.51	0/44	0.67	0/60
All	All	0.49	0/8387	0.72	1/11345 (0.0%)

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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	677	LYS	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	693	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2014	0	2033	248	0
1	B	1997	0	2014	222	0
1	C	2014	0	2033	273	0
1	D	2014	0	2033	237	0
2	E	45	0	20	1	0
2	F	45	0	20	5	0
2	G	45	0	20	3	0
2	H	45	0	20	2	0
3	A	28	0	28	1	0
3	B	28	0	28	3	0
3	C	28	0	27	2	0
3	D	28	0	28	5	0
All	All	8331	0	8304	962	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 58.

The worst 5 of 962 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:A:761:ILE:HB	1:A:762:PRO:HD3	1.22	1.13
1:C:677:LYS:HE3	1:C:770:LYS:HB2	1.34	1.09
1:A:531:THR:HG22	1:A:533:VAL:H	1.19	1.05
1:B:531:THR:HG22	1:B:532:LEU:H	1.23	1.03
1:A:761:ILE:HB	1:A:762:PRO:CD	1.92	0.98

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	243/280 (87%)	190 (78%)	34 (14%)	19 (8%)	1	1
1	B	241/280 (86%)	185 (77%)	35 (14%)	21 (9%)	1	1
1	C	243/280 (87%)	172 (71%)	51 (21%)	20 (8%)	1	1
1	D	243/280 (87%)	181 (74%)	39 (16%)	23 (10%)	0	0
2	E	7/12 (58%)	5 (71%)	2 (29%)	0	100	100
2	F	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
2	G	7/12 (58%)	7 (100%)	0	0	100	100
2	H	7/12 (58%)	7 (100%)	0	0	100	100
All	All	998/1168 (85%)	753 (76%)	162 (16%)	83 (8%)	1	1

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	676	PRO
1	A	709	SER
1	A	711	ASN
1	A	761	ILE
1	B	551	SER

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	227/255 (89%)	203 (89%)	24 (11%)	6	15
1	B	225/255 (88%)	195 (87%)	30 (13%)	4	9
1	C	227/255 (89%)	201 (88%)	26 (12%)	5	13
1	D	227/255 (89%)	200 (88%)	27 (12%)	5	12
All	All	906/1020 (89%)	799 (88%)	107 (12%)	5	12

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	553	PRO
1	C	710	GLN
1	D	710	GLN
1	C	585	ARG
1	C	641	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	776	GLN
1	D	768	ASN
1	D	586	ASN
1	D	657	GLN
1	B	632	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	DEX	B	2999	-	31,31,31	4.21	23 (74%)	52,53,53	3.11	22 (42%)
3	DEX	C	3999	-	31,31,31	4.41	22 (70%)	52,53,53	3.29	23 (44%)
3	DEX	A	1999	-	31,31,31	4.35	23 (74%)	52,53,53	3.10	22 (42%)
3	DEX	D	4999	-	31,31,31	4.25	23 (74%)	52,53,53	3.01	23 (44%)

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	B	2999	-	-	6/8/84/84	0/4/4/4
3	DEX	C	3999	-	-	6/8/84/84	0/4/4/4
3	DEX	A	1999	-	-	6/8/84/84	0/4/4/4
3	DEX	D	4999	-	-	6/8/84/84	0/4/4/4

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2999	DEX	C10-C1	9.19	1.61	1.50
3	A	1999	DEX	C10-C1	9.11	1.61	1.50
3	C	3999	DEX	C10-C1	8.67	1.60	1.50
3	C	3999	DEX	C9-C11	8.53	1.62	1.54
3	A	1999	DEX	C6-C5	8.19	1.64	1.50

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3999	DEX	C12-C13-C17	10.32	124.02	115.57
3	B	2999	DEX	C12-C13-C17	9.97	123.73	115.57
3	A	1999	DEX	C12-C13-C17	9.35	123.23	115.57
3	D	4999	DEX	C12-C13-C17	9.27	123.17	115.57
3	A	1999	DEX	O3-C17-C20	-6.79	91.58	107.04

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1999	DEX	C13-C17-C20-C21
3	A	1999	DEX	C13-C17-C20-O4

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Mol	Chain	Res	Type	Atoms
3	A	1999	DEX	C16-C17-C20-C21
3	A	1999	DEX	C16-C17-C20-O4
3	A	1999	DEX	O3-C17-C20-C21

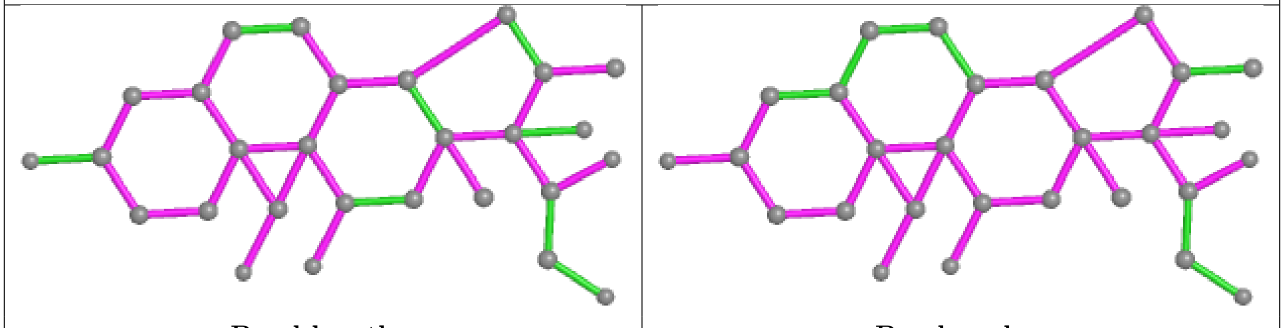
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2999	DEX	3	0
3	C	3999	DEX	2	0
3	A	1999	DEX	1	0
3	D	4999	DEX	5	0

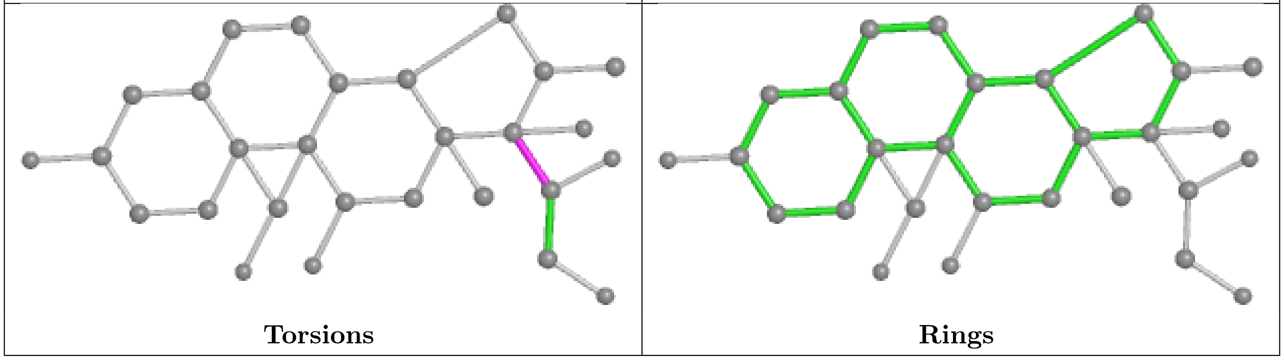
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand DEX B 2999



Bond lengths

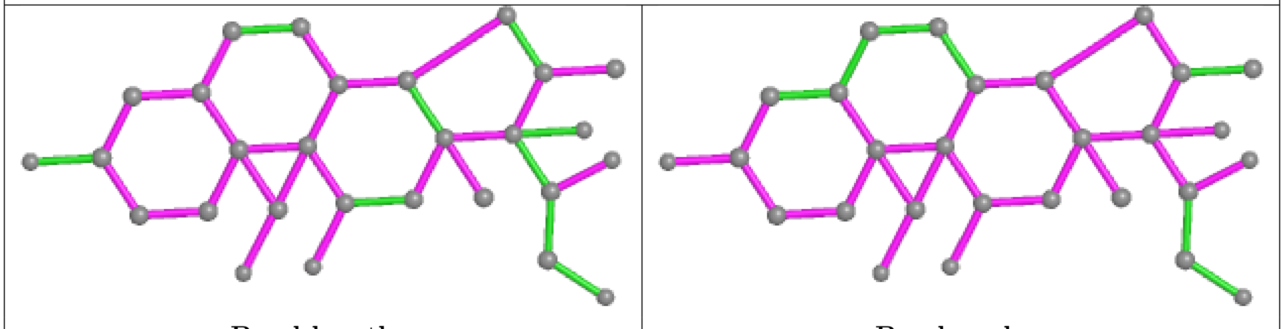
Bond angles



Torsions

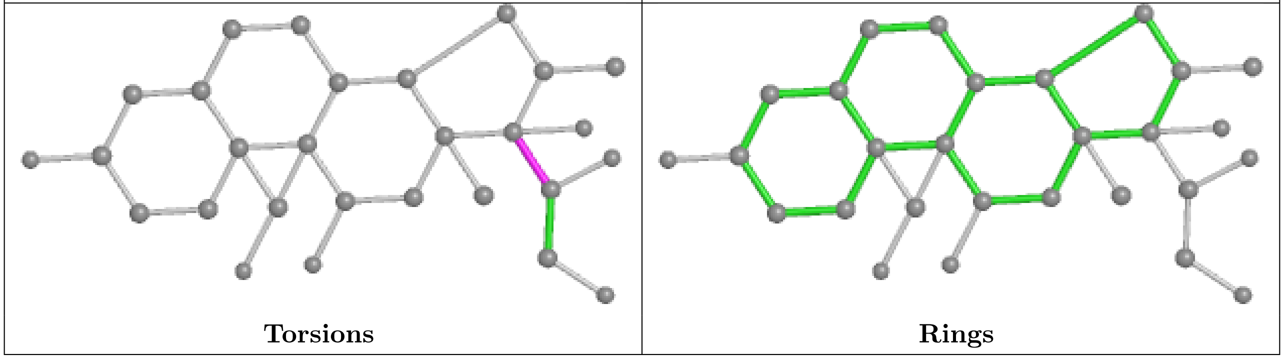
Rings

Ligand DEX C 3999



Bond lengths

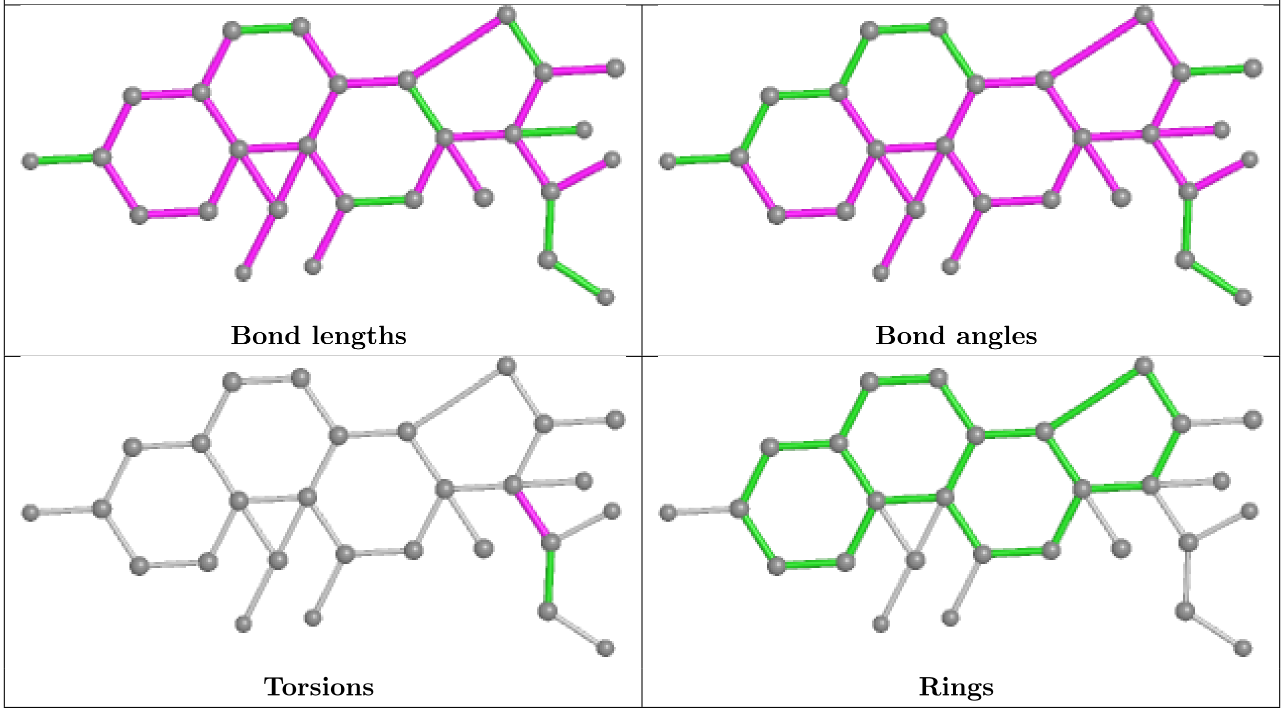
Bond angles



Torsions

Rings

Ligand DEX A 1999



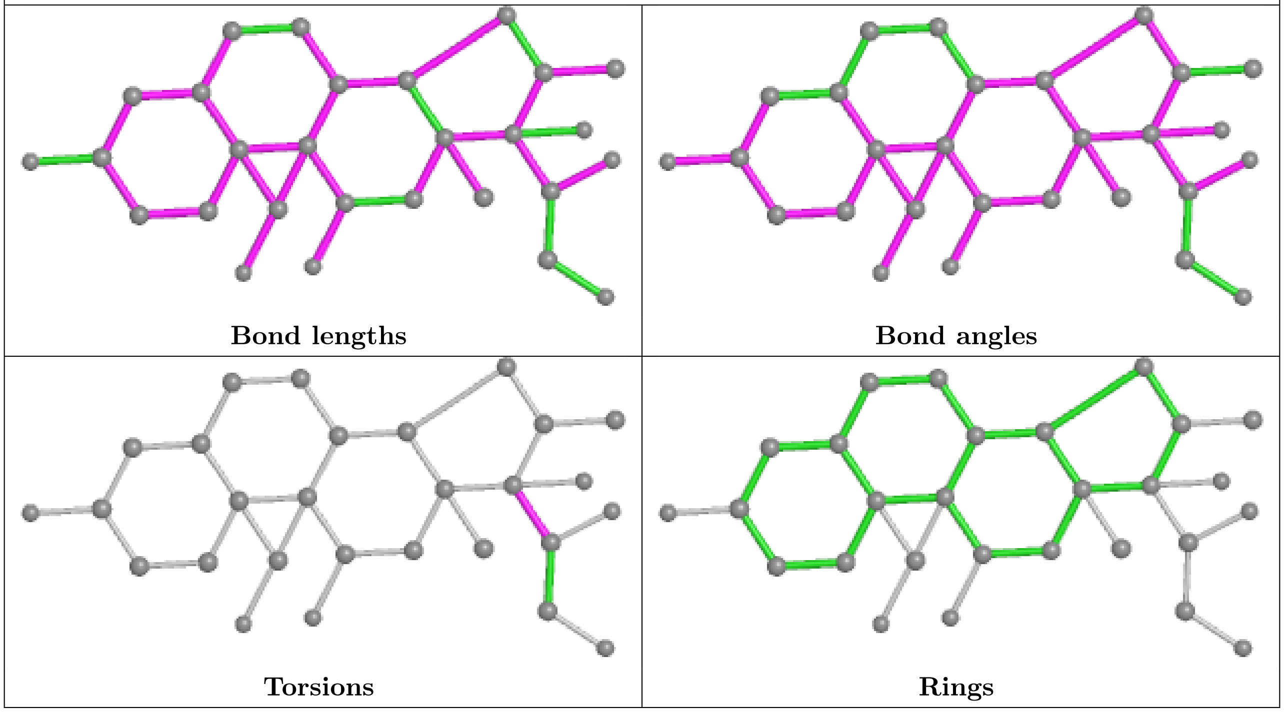
Bond lengths

Bond angles

Torsions

Rings

Ligand DEX D 4999



Bond lengths

Bond angles

Torsions

Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

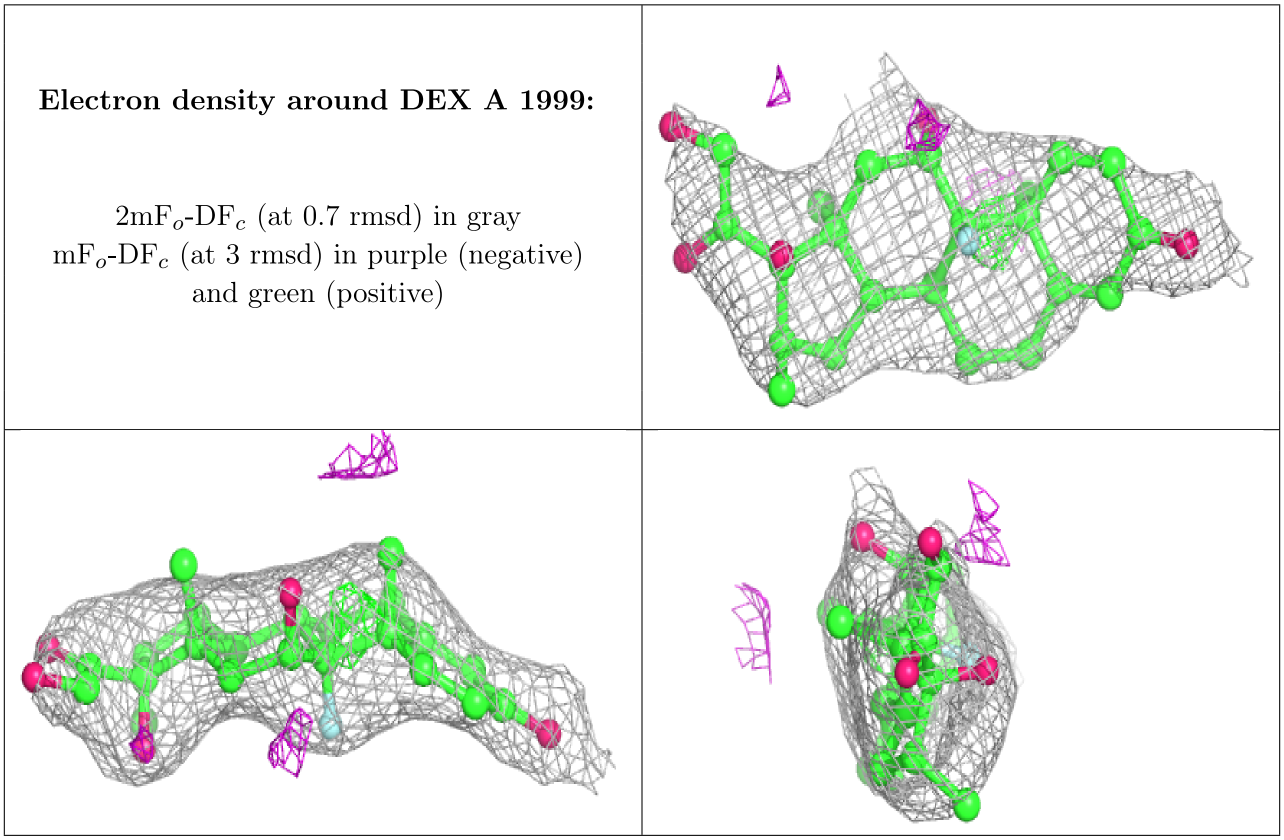
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

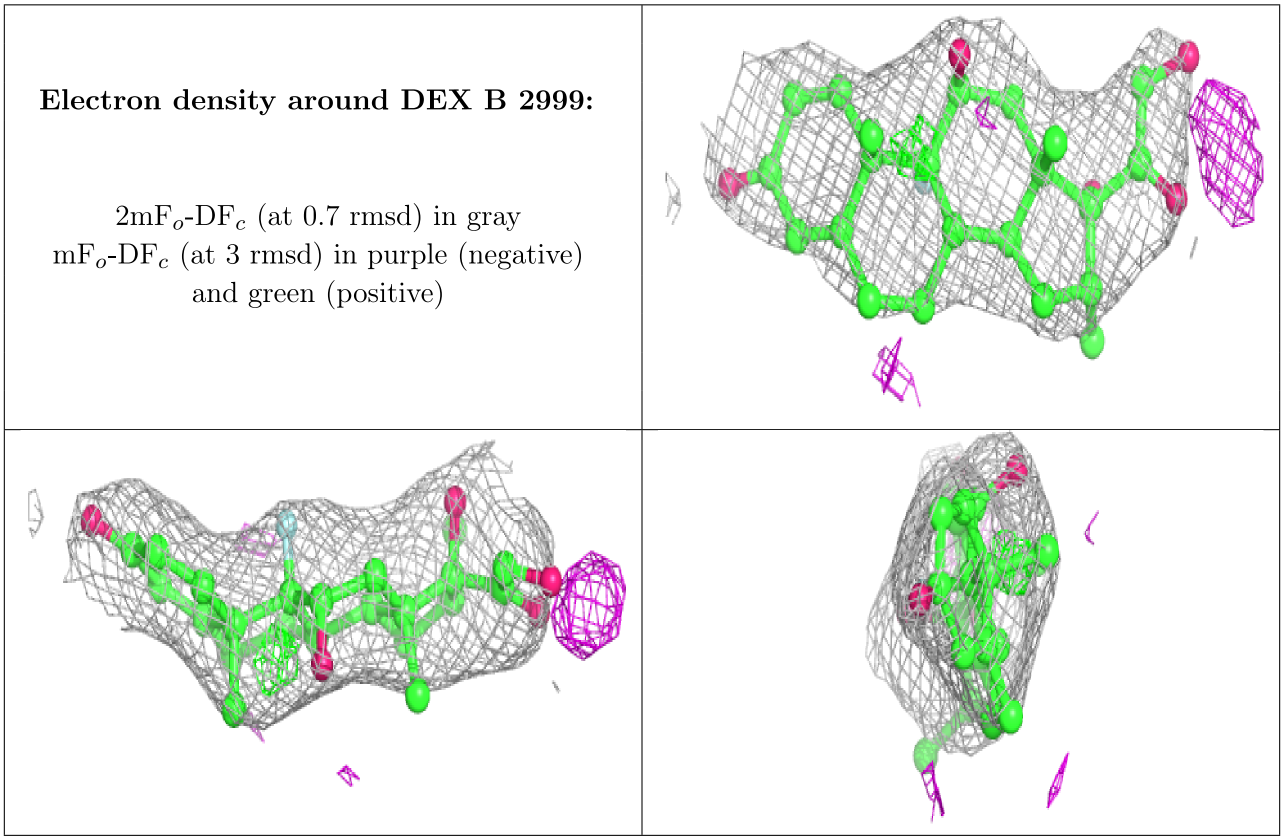


Electron density around DEX A 1999:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

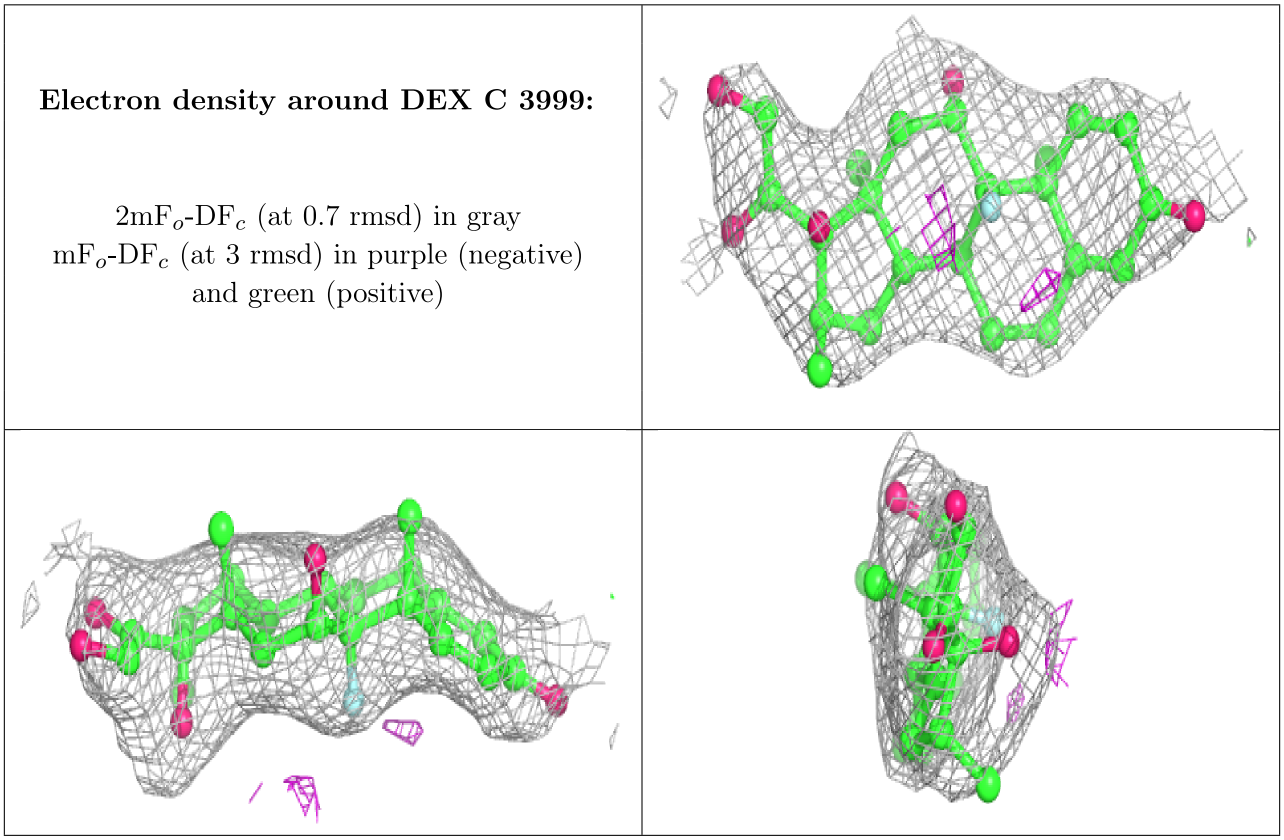
Electron density around DEX B 2999:

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



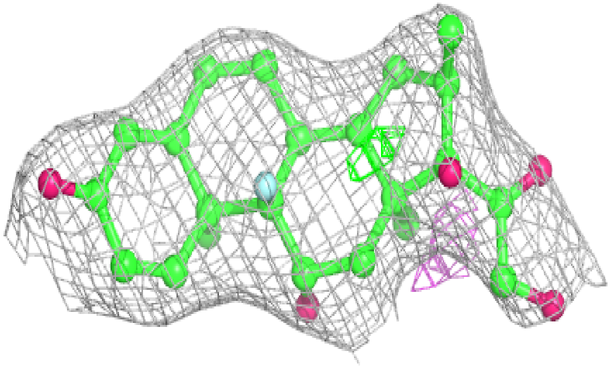
Electron density around DEX C 3999:

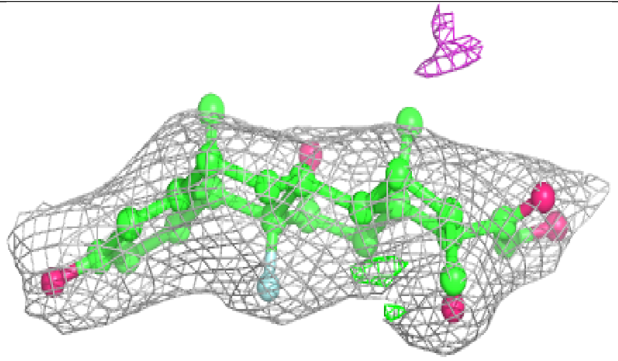
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

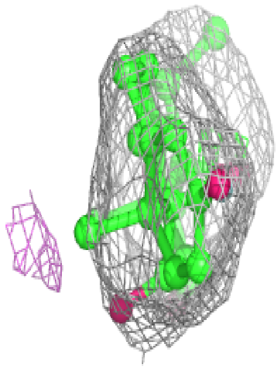


Electron density around DEX D 4999:

$2mF_o$-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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.