Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 12:34 am GMT

PDB ID	:	7YXD
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	:	2022-02-15
Resolution	:	2.30 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:

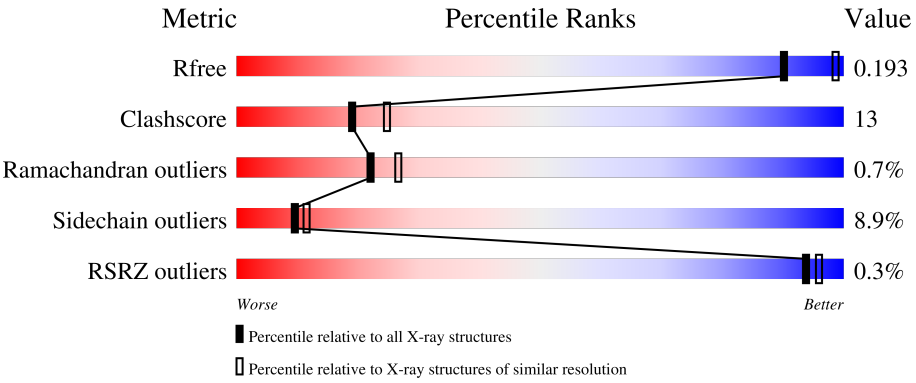
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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	A	248	69% 25%
1	D	248	71% 22%
1	H	248	69% 24%
1	L	248	70% 23%
2	C	12	50% 42% 8%

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Mol	Chain	Length	Quality of chain
2	F	12	58% 33% 8%
2	J	12	8% 50% 25% 17% 8%
2	N	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.

- Molecule 1 is a protein called Ancestral Glucocorticoid Receptor2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	1	0
			1958	1271	318	351	18			
1	D	240	Total	C	N	O	S	0	1	0
			1946	1261	317	350	18			
1	H	241	Total	C	N	O	S	0	0	0
			1956	1270	318	351	17			
1	L	241	Total	C	N	O	S	0	1	0
			1957	1270	318	351	18			

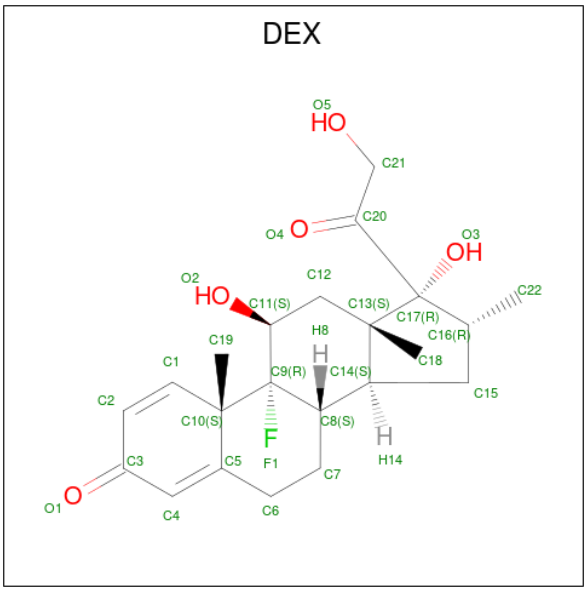
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	529	PHE	-	expression tag	UNP A0A1X8XLE9
D	529	PHE	-	expression tag	UNP A0A1X8XLE9
H	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	C	11	Total	C	N	O	0	0	0
			84	56	14	14			
2	F	11	Total	C	N	O	0	0	0
			84	56	14	14			
2	J	12	Total	C	N	O	0	0	0
			90	59	15	16			
2	N	11	Total	C	N	O	0	0	0
			84	56	14	14			

- 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	A	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	H	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	H	1	Total Na 1 1	0	0

- Molecule 5 is water.

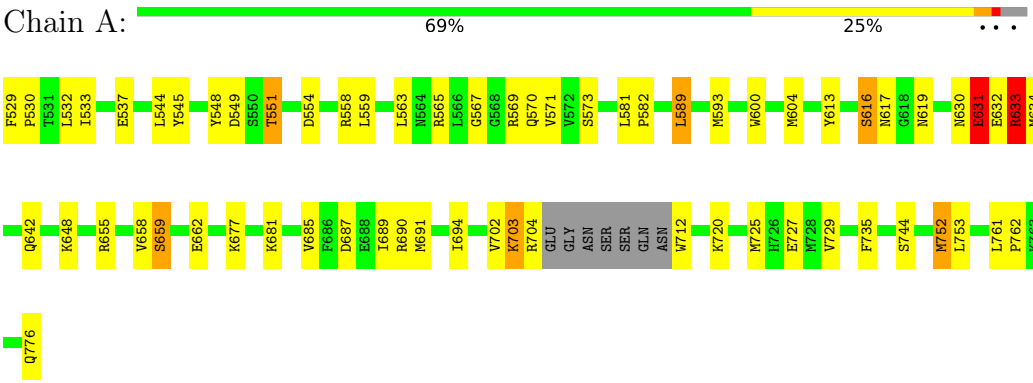
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	D	1	Total O 1 1	0	0
5	H	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0

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.

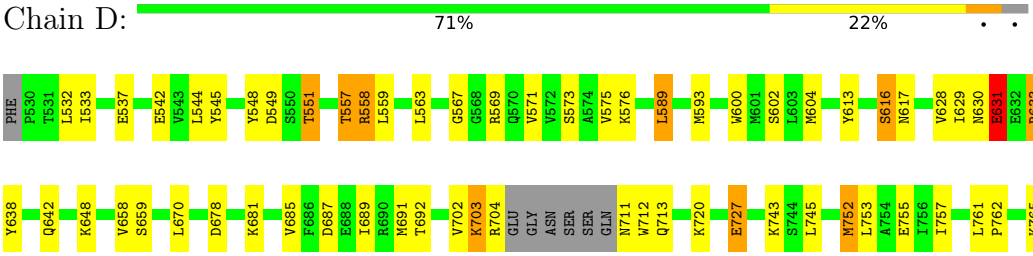
• Molecule 1: Ancestral Glucocorticoid Receptor2

Chain A:



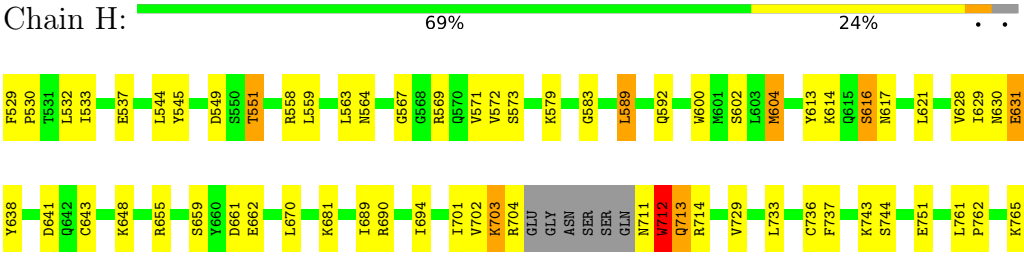
• Molecule 1: Ancestral Glucocorticoid Receptor2

Chain D:



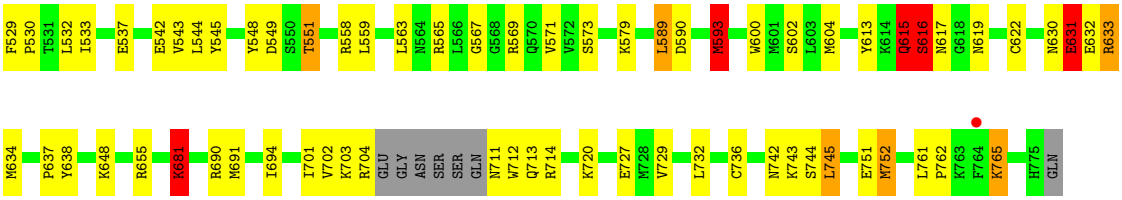
• Molecule 1: Ancestral Glucocorticoid Receptor2

Chain H:



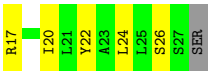
• Molecule 1: Ancestral Glucocorticoid Receptor2

Chain L:



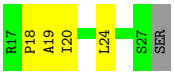
• Molecule 2: SHP NR Box 1 Peptide

Chain C:



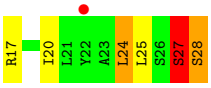
• Molecule 2: SHP NR Box 1 Peptide

Chain F:



• Molecule 2: SHP NR Box 1 Peptide

Chain J:



• Molecule 2: SHP NR Box 1 Peptide

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	107.60Å 107.60Å 135.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.81 – 2.30 76.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.4 (76.81-2.30) 94.4 (76.81-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.221 0.149 , 0.193	Depositor 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[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.450 for -h,-k,l 0.449 for h,-h-k,-l 0.449 for -k,-h,-l	Xtriage
Reported twinning fraction	0.265 for H, K, L 0.240 for K, H, -L 0.237 for -K, -H, -L 0.259 for -h,-k,l	Depositor
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.*

[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, 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	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	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	H	0.53	0/1999	1.01	2/2698 (0.1%)
1	L	0.53	0/2005	1.04	6/2706 (0.2%)
2	C	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	N	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	A	0	2
1	D	0	1
1	H	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)	Ideal(Å)
1	D	631	GLU	CD-OE2	7.50	1.33	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	681	LYS	CB-CA-C	6.60	123.61	110.40
1	A	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
1	D	633	ARG	CG-CD-NE	-5.55	100.14	111.80
1	L	593	MET	N-CA-CB	-5.52	100.67	110.60
1	L	729	VAL	CA-CB-CG1	5.51	119.17	110.90
1	D	727	GLU	CB-CG-CD	5.50	129.04	114.20
1	H	572	VAL	CA-CB-CG2	5.33	118.89	110.90
1	H	733	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	L	743	LYS	CB-CA-C	5.01	120.41	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	631	GLU	Peptide
1	A	712	TRP	Peptide
1	D	631	GLU	Peptide
1	H	631	GLU	Peptide
2	J	27	SER	Peptide
1	L	615	GLN	Peptide
1	L	631	GLU	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	A	1958	0	1991	50	0
1	D	1946	0	1981	55	0
1	H	1956	0	1986	57	0
1	L	1957	0	1989	45	0
2	C	84	0	92	10	0
2	F	84	0	92	11	0
2	J	90	0	97	9	0
2	N	84	0	92	8	0
3	A	28	0	29	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	29	3	0
3	H	28	0	29	5	0
3	L	28	0	29	3	0
4	H	1	0	0	0	0
5	A	4	0	0	0	0
5	D	1	0	0	0	0
5	H	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.

All (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
1:L:616:SER:O	1:L:619:ASN:ND2	2.07	0.86
1:D:630:ASN:O	1:D:633:ARG:N	2.10	0.85
1:A:631:GLU:HB3	1:A:634:MET:HE2	1.58	0.84
1:A:593:MET:HE2	2:C:22:TYR:CD1	2.14	0.82
1:H:765:LYS:NZ	1:L:765:LYS:O	2.11	0.80
1:A:633:ARG:O	1:A:633:ARG:HG2	1.80	0.80
1:H:631:GLU:OE1	1:H:634:MET:HE2	1.82	0.80
1:A:589:LEU:HD11	2:C:26:SER:HB3	1.62	0.79
1:D:703:LYS:HG2	1:D:703:LYS:O	1.82	0.79
1:H:630:ASN:OD1	1:H:633:ARG:HG2	1.83	0.79
1:H:703:LYS:O	1:H:703:LYS:HG2	1.81	0.79
1:H:564:ASN:OD1	3:H:1001:DEX:H211	1.83	0.78
1:D:557:THR:HG21	1:D:745:LEU:O	1.83	0.77
1:D:575:VAL:HG11	2:F:24:LEU:HB3	1.66	0.77
1:D:659:SER:HB2	1:D:704:ARG:HD2	1.66	0.77
1:H:711:ASN:O	1:H:712:TRP:C	2.22	0.77
1:H:630:ASN:OD1	1:H:633:ARG:CG	2.34	0.76
1:L:630:ASN:OD1	1:L:633:ARG:CG	2.32	0.76
1:L:579:LYS:HD2	2:N:25:LEU:HD23	1.66	0.76
1:L:593:MET:HE3	2:N:22:TYR:CD1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:GLU:HA	1:D:634:MET:H	1.52	0.74
1:H:631:GLU:OE1	1:H:634:MET:CE	2.36	0.74
1:D:557:THR:CG2	1:D:745:LEU:O	2.36	0.74
1:D:593:MET:SD	2:F:18:PRO:HD2	2.28	0.74
2:C:20:ILE:O	2:C:24:LEU:HD23	1.88	0.73
1:L:702:VAL:C	1:L:704:ARG:H	1.91	0.73
1:L:742:ASN:OD1	1:L:745:LEU:HB2	1.88	0.73
1:A:703:LYS:O	1:A:703:LYS:HG2	1.88	0.72
1:H:702:VAL:C	1:H:704:ARG:H	1.92	0.71
1:A:633:ARG:O	1:A:633:ARG:CG	2.38	0.71
1:H:659:SER:HB2	1:H:704:ARG:HD2	1.73	0.70
1:H:589:LEU:HD23	1:H:592:GLN:OE1	1.92	0.69
1:H:641:ASP:CG	1:L:742:ASN:HD21	1.94	0.69
1:A:593:MET:CE	2:C:22:TYR:HB2	2.22	0.68
1:D:631:GLU:HG2	1:D:634:MET:HE2	1.74	0.68
2:F:20:ILE:O	2:F:24:LEU:HD23	1.92	0.68
1:D:752:MET:SD	2:F:20:ILE:CG2	2.81	0.68
1:D:752:MET:SD	2:F:20:ILE:HB	2.32	0.68
1:H:690:ARG:O	1:H:694:ILE:HG13	1.93	0.68
1:A:690:ARG:O	1:A:694:ILE:HG13	1.93	0.68
2:N:20:ILE:O	2:N:24:LEU:HD23	1.94	0.68
1:A:633:ARG:HG3	1:A:636:LEU:HD12	1.75	0.66
1:H:711:ASN:C	1:H:713:GLN:N	2.42	0.66
2:J:27:SER:HB3	2:J:28:SER:HB2	1.79	0.65
1:D:711:ASN:OD1	1:D:711:ASN:O	2.16	0.64
1:A:589:LEU:CD1	2:C:26:SER:HB3	2.28	0.64
1:L:711:ASN:OD1	1:L:712:TRP:HD1	1.81	0.64
1:L:702:VAL:O	1:L:704:ARG:N	2.30	0.64
1:H:702:VAL:O	1:H:704:ARG:N	2.30	0.63
1:A:702:VAL:C	1:A:704:ARG:H	2.01	0.63
1:L:630:ASN:O	1:L:633:ARG:N	2.30	0.63
2:J:20:ILE:HG22	2:J:24:LEU:CD2	2.29	0.62
1:A:570:GLN:OE1	3:A:1001:DEX:H2	2.00	0.61
1:L:690:ARG:O	1:L:694:ILE:HG13	2.00	0.61
1:A:630:ASN:O	1:A:633:ARG:N	2.33	0.61
1:H:661:ASP:OD1	1:H:703:LYS:HE2	1.99	0.61
1:A:685:VAL:O	1:A:689:ILE:HG12	2.01	0.60
1:H:701:ILE:HG12	1:H:714:ARG:HG3	1.83	0.60
3:H:1001:DEX:O2	3:H:1001:DEX:H931	2.01	0.60
3:A:1001:DEX:H821	3:A:1001:DEX:O2	2.02	0.59
1:H:579:LYS:HD2	2:J:25:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLN:OE1	3:A:1001:DEX:C2	2.52	0.58
1:A:600:TRP:O	1:A:604:MET:HG2	2.04	0.58
1:D:702:VAL:C	1:D:704:ARG:H	2.06	0.58
1:L:549:ASP:OD1	1:L:551:THR:HB	2.03	0.58
1:L:593:MET:CE	2:N:22:TYR:HD1	2.16	0.57
1:A:589:LEU:HD11	2:C:26:SER:CB	2.34	0.56
1:H:579:LYS:HZ2	2:J:25:LEU:C	2.08	0.56
1:D:630:ASN:O	1:D:633:ARG:CA	2.53	0.56
1:H:567:GLY:O	1:H:571:VAL:HG23	2.05	0.56
1:L:590:ASP:OD2	2:N:17:ARG:NH1	2.38	0.56
1:H:630:ASN:OD1	1:H:633:ARG:HG3	2.04	0.55
1:H:630:ASN:O	1:H:633:ARG:N	2.38	0.55
1:L:579:LYS:HE3	2:N:25:LEU:O	2.07	0.55
1:L:545:TYR:O	1:L:569:ARG:NH1	2.30	0.55
1:L:702:VAL:C	1:L:704:ARG:N	2.60	0.54
1:L:593:MET:HE3	2:N:22:TYR:HD1	1.66	0.54
1:A:593:MET:SD	2:C:22:TYR:HA	2.46	0.54
1:L:567:GLY:O	1:L:571:VAL:HG23	2.07	0.54
2:J:20:ILE:O	2:J:24:LEU:CD2	2.56	0.54
3:D:1001:DEX:H821	3:D:1001:DEX:O2	2.08	0.54
2:J:20:ILE:O	2:J:24:LEU:HD22	2.08	0.54
1:D:752:MET:SD	2:F:20:ILE:CB	2.95	0.53
1:H:702:VAL:C	1:H:704:ARG:N	2.60	0.53
1:D:642:GLN:HB2	3:D:1001:DEX:C22	2.39	0.53
1:H:549:ASP:OD1	1:H:551:THR:HB	2.09	0.53
1:D:642:GLN:HB2	3:D:1001:DEX:H222	1.91	0.53
1:H:579:LYS:HD2	2:J:25:LEU:HA	1.89	0.53
1:H:761:LEU:O	1:H:765:LYS:HG3	2.09	0.53
1:H:563:LEU:HB3	3:H:1001:DEX:H11	1.90	0.53
1:D:549:ASP:OD1	1:D:551:THR:HB	2.08	0.52
1:H:637:PRO:O	1:H:638:TYR:HB2	2.10	0.52
1:H:661:ASP:OD1	1:H:703:LYS:CE	2.58	0.52
1:L:681:LYS:HD2	1:L:681:LYS:N	2.24	0.52
1:D:544:LEU:HD13	1:D:569:ARG:HB3	1.92	0.52
1:L:637:PRO:O	1:L:638:TYR:HB2	2.08	0.52
1:D:631:GLU:HG2	1:D:634:MET:HG3	1.92	0.52
1:A:655:ARG:HG2	1:A:655:ARG:HH11	1.74	0.51
1:L:615:GLN:O	1:L:622[B]:CYS:SG	2.65	0.51
1:D:685:VAL:O	1:D:689:ILE:HG12	2.11	0.51
1:A:545:TYR:O	1:A:569:ARG:NH1	2.30	0.51
1:A:567:GLY:O	1:A:571:VAL:HG23	2.11	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	2.10	0.51
1:A:549:ASP:OD1	1:A:551:THR:HB	2.12	0.50
1:D:755:GLU:CD	2:F:20:ILE:HD12	2.31	0.50
1:H:602:SER:OG	1:H:729:VAL:HG11	2.11	0.50
1:L:761:LEU:HB3	1:L:762:PRO:HD3	1.94	0.50
1:A:703:LYS:O	1:A:703:LYS:CG	2.59	0.50
1:D:631:GLU:HA	1:D:634:MET:HB2	1.93	0.50
1:D:633:ARG:HG2	1:D:636:LEU:CD1	2.42	0.50
1:H:600:TRP:O	1:H:604:MET:CG	2.55	0.49
1:D:567:GLY:O	1:D:571:VAL:HG23	2.12	0.49
1:H:736:CYS:HA	3:H:1001:DEX:O4	2.12	0.49
1:A:593:MET:CE	2:C:22:TYR:CB	2.89	0.49
1:D:533:ILE:O	1:D:537:GLU:HG3	2.12	0.49
1:L:701:ILE:HG12	1:L:714:ARG:HG3	1.94	0.49
1:H:662:GLU:OE1	1:H:714:ARG:NH2	2.46	0.49
1:L:571:VAL:HG12	1:L:752:MET:CE	2.42	0.49
1:L:533:ILE:O	1:L:537:GLU:HG3	2.13	0.49
1:D:631:GLU:HA	1:D:634:MET:N	2.26	0.48
1:L:590:ASP:CG	2:N:17:ARG:HH12	2.16	0.48
3:H:1001:DEX:O2	3:H:1001:DEX:C19	2.61	0.48
1:H:589:LEU:CD2	1:H:592:GLN:OE1	2.61	0.48
1:L:571:VAL:HG12	1:L:752:MET:HE2	1.94	0.48
1:A:659:SER:OG	1:A:704:ARG:HD2	2.13	0.48
1:H:559:LEU:O	1:H:563:LEU:HG	2.14	0.48
1:D:545:TYR:O	1:D:569:ARG:NH1	2.33	0.48
1:D:637:PRO:O	1:D:638:TYR:HB2	2.14	0.48
1:A:533:ILE:O	1:A:537:GLU:HG3	2.14	0.47
1:H:703:LYS:O	1:H:703:LYS:CG	2.58	0.47
1:A:761:LEU:HB3	1:A:762:PRO:HD3	1.97	0.47
1:D:761:LEU:HB3	1:D:762:PRO:HD3	1.95	0.47
1:H:631:GLU:OE1	1:H:634:MET:HE1	2.12	0.47
1:L:589:LEU:HD22	1:L:589:LEU:HA	1.70	0.46
1:A:765:LYS:HG2	1:D:765:LYS:O	2.15	0.46
1:D:753:LEU:HD23	1:D:753:LEU:HA	1.72	0.46
1:D:600:TRP:O	1:D:604:MET:HG2	2.16	0.46
1:L:600:TRP:O	1:L:604:MET:HG2	2.16	0.46
1:A:548:TYR:OH	1:A:554:ASP:OD1	2.22	0.46
3:A:1001:DEX:O2	3:A:1001:DEX:C18	2.63	0.46
1:D:752:MET:SD	2:F:20:ILE:HG22	2.55	0.46
1:D:548:TYR:CE2	1:D:633:ARG:NH1	2.84	0.46
1:D:631:GLU:HG2	1:D:634:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:LEU:O	1:D:563:LEU:HG	2.16	0.46
1:L:711:ASN:OD1	1:L:712:TRP:N	2.49	0.46
1:H:711:ASN:OD1	1:H:712:TRP:N	2.49	0.45
1:L:616:SER:O	1:L:616:SER:OG	2.34	0.45
1:L:655:ARG:HH11	1:L:655:ARG:HG2	1.81	0.45
1:A:631:GLU:HB3	1:A:634:MET:CE	2.39	0.45
1:A:702:VAL:C	1:A:704:ARG:N	2.68	0.45
1:D:755:GLU:OE2	2:F:19:ALA:N	2.49	0.45
1:A:616:SER:O	1:A:616:SER:OG	2.33	0.45
1:D:589:LEU:HD22	1:D:589:LEU:HA	1.83	0.45
1:L:548:TYR:HE2	1:L:633:ARG:HH12	1.64	0.45
1:A:559:LEU:O	1:A:563:LEU:HG	2.17	0.45
1:A:687:ASP:O	1:A:691:MET:HG3	2.16	0.45
1:D:755:GLU:OE1	2:F:20:ILE:HD12	2.16	0.45
1:H:544:LEU:HD13	1:H:569:ARG:HB3	1.98	0.45
1:H:583:GLY:O	1:H:689:ILE:HD11	2.17	0.45
1:H:761:LEU:HB3	1:H:762:PRO:HD3	1.97	0.45
1:A:752:MET:HA	2:C:20:ILE:HD12	1.99	0.45
1:D:755:GLU:OE1	2:F:20:ILE:CD1	2.64	0.45
1:A:725:MET:O	1:A:729:VAL:HB	2.17	0.45
1:D:549:ASP:O	1:D:558:ARG:NH2	2.50	0.44
1:D:703:LYS:O	1:D:703:LYS:CG	2.61	0.44
1:H:616:SER:O	1:H:616:SER:OG	2.33	0.44
1:H:628:VAL:HG12	1:H:629:ILE:N	2.32	0.44
2:J:27:SER:HB3	2:J:28:SER:CB	2.46	0.44
1:D:631:GLU:CA	1:D:634:MET:H	2.27	0.44
1:H:533:ILE:O	1:H:537:GLU:HG3	2.16	0.44
1:A:753:LEU:HD23	1:A:753:LEU:HA	1.68	0.44
1:D:757:ILE:HD13	1:D:757:ILE:HG21	1.77	0.44
1:L:631:GLU:OE1	1:L:634:MET:SD	2.76	0.44
1:H:737:PHE:CG	1:H:761:LEU:HD13	2.53	0.44
3:L:1001:DEX:O4	3:L:1001:DEX:C18	2.65	0.44
1:A:549:ASP:O	1:A:558:ARG:NH2	2.50	0.43
1:D:670:LEU:HD23	1:D:670:LEU:HA	1.89	0.43
1:H:545:TYR:O	1:H:569:ARG:NH1	2.30	0.43
1:H:655:ARG:HG2	1:H:655:ARG:HH11	1.83	0.43
1:L:549:ASP:O	1:L:558:ARG:NH2	2.50	0.43
1:H:621:LEU:HD12	1:H:643:CYS:SG	2.58	0.43
1:D:613:TYR:O	1:D:617:ASN:HA	2.18	0.43
1:A:677:LYS:HA	1:A:770:LYS:HE3	2.01	0.43
1:D:548:TYR:HE2	1:D:633:ARG:NH1	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:559:LEU:O	1:L:563:LEU:HG	2.19	0.43
1:L:736:CYS:HA	3:L:1001:DEX:O4	2.19	0.43
1:A:642:GLN:NE2	1:A:735:PHE:CE1	2.88	0.42
1:A:529:PHE:N	1:A:530:PRO:CD	2.82	0.42
1:A:613:TYR:O	1:A:617:ASN:HA	2.20	0.42
3:L:1001:DEX:O4	3:L:1001:DEX:H831	2.18	0.42
1:D:658:VAL:HG12	1:D:659:SER:O	2.20	0.42
1:A:659:SER:OG	1:A:662:GLU:CD	2.58	0.42
1:A:658:VAL:HG12	1:A:659:SER:O	2.19	0.42
1:D:633:ARG:HG2	1:D:636:LEU:HD12	2.00	0.42
1:H:670:LEU:HD23	1:H:670:LEU:HA	1.87	0.42
1:L:543:VAL:HG22	1:L:544:LEU:O	2.20	0.42
1:D:687:ASP:O	1:D:691:MET:HG3	2.20	0.42
1:L:529:PHE:N	1:L:530:PRO:CD	2.83	0.41
1:H:529:PHE:N	1:H:530:PRO:CD	2.83	0.41
1:H:613:TYR:O	1:H:617:ASN:HA	2.20	0.41
1:H:712:TRP:O	1:H:713:GLN:C	2.59	0.41
1:D:659:SER:CB	1:D:704:ARG:HD2	2.43	0.41
1:L:613:TYR:O	1:L:617:ASN:HA	2.20	0.41
1:A:581:LEU:O	1:A:582:PRO:C	2.59	0.41
1:D:628:VAL:HG12	1:D:629:ILE:N	2.36	0.41
1:A:544:LEU:HD13	1:A:569:ARG:HB3	2.03	0.41
1:D:631:GLU:HG2	1:D:634:MET:CG	2.50	0.41
1:H:549:ASP:O	1:H:558:ARG:NH2	2.51	0.41
1:A:631:GLU:H	1:A:631:GLU:HG3	1.48	0.40
1:A:616:SER:O	1:A:619:ASN:ND2	2.54	0.40
1:D:616:SER:O	1:D:616:SER:OG	2.32	0.40
1:H:579:LYS:NZ	2:J:25:LEU:O	2.41	0.40
1:L:701:ILE:HG12	1:L:714:ARG:CG	2.51	0.40

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	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	H	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	C	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	N	9/12 (75%)	9 (100%)	0	0	100 100
All	All	987/1040 (95%)	947 (96%)	33 (3%)	7 (1%)	22 26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	712	TRP
1	L	616	SER
1	D	703	LYS
1	H	703	LYS
1	L	703	LYS
1	A	631	GLU
1	A	703	LYS

5.3.2 Protein sidechains (i)

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	222/227 (98%)	205 (92%)	17 (8%)	13 16
1	D	221/227 (97%)	202 (91%)	19 (9%)	10 12
1	H	221/227 (97%)	205 (93%)	16 (7%)	14 18
1	L	222/227 (98%)	198 (89%)	24 (11%)	6 7
2	C	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 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	9/10 (90%)	8 (89%)	1 (11%)	6 7
All	All	923/948 (97%)	841 (91%)	82 (9%)	9 11

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	LEU
1	A	551	THR
1	A	565	ARG
1	A	573	SER
1	A	589	LEU
1	A	616	SER
1	A	631	GLU
1	A	632	GLU
1	A	633	ARG
1	A	648	LYS
1	A	659	SER
1	A	681	LYS
1	A	720	LYS
1	A	727	GLU
1	A	744	SER
1	A	752	MET
1	A	776	GLN
2	C	17	ARG
1	D	532	LEU
1	D	542	GLU
1	D	551	THR
1	D	557	THR
1	D	558	ARG
1	D	573	SER
1	D	576	LYS
1	D	589	LEU
1	D	602	SER
1	D	616	SER
1	D	648	LYS
1	D	678	ASP
1	D	681	LYS
1	D	712	TRP
1	D	713	GLN
1	D	720	LYS
1	D	727	GLU
1	D	743	LYS

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Mol	Chain	Res	Type
1	D	752	MET
1	H	532	LEU
1	H	551	THR
1	H	573	SER
1	H	589	LEU
1	H	604	MET
1	H	614	LYS
1	H	616	SER
1	H	632	GLU
1	H	633	ARG
1	H	648	LYS
1	H	681	LYS
1	H	712	TRP
1	H	713	GLN
1	H	743	LYS
1	H	744	SER
1	H	751	GLU
2	J	17	ARG
2	J	24	LEU
2	J	27	SER
2	J	28	SER
1	L	532	LEU
1	L	542	GLU
1	L	551	THR
1	L	565	ARG
1	L	573	SER
1	L	589	LEU
1	L	593	MET
1	L	602	SER
1	L	615	GLN
1	L	616	SER
1	L	631	GLU
1	L	632	GLU
1	L	633	ARG
1	L	648	LYS
1	L	681	LYS
1	L	691	MET
1	L	713	GLN
1	L	720	LYS
1	L	727	GLU
1	L	744	SER
1	L	745	LEU

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Mol	Chain	Res	Type
1	L	751	GLU
1	L	752	MET
1	L	765	LYS
2	N	17	ARG

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

Mol	Chain	Res	Type
1	A	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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					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	H	1001	-	31,31,31	0.63	0	52,53,53	2.50	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	DEX	A	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	H	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.

All (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	H	1001	DEX	O2-C11-C9	-6.58	99.35	109.08
3	A	1001	DEX	C19-C10-C9	6.37	118.11	113.55
3	A	1001	DEX	C13-C17-C20	-6.26	106.25	112.89
3	H	1001	DEX	C6-C5-C10	6.02	119.32	115.61
3	H	1001	DEX	F1-C9-C8	-5.53	100.98	105.95
3	H	1001	DEX	C12-C11-C9	5.31	116.64	112.93
3	D	1001	DEX	F1-C9-C10	-4.95	99.99	104.19
3	A	1001	DEX	C10-C9-C11	4.75	119.00	115.52
3	H	1001	DEX	F1-C9-C11	4.47	106.61	102.72
3	D	1001	DEX	C12-C13-C17	4.36	119.14	115.57
3	L	1001	DEX	O2-C11-C9	-4.33	102.68	109.08
3	D	1001	DEX	C1-C2-C3	-4.26	117.84	121.47
3	H	1001	DEX	C9-C8-C14	-4.16	106.02	109.26
3	D	1001	DEX	C10-C9-C11	4.15	118.56	115.52
3	H	1001	DEX	C10-C9-C11	-4.12	112.50	115.52
3	D	1001	DEX	C1-C10-C5	-4.10	110.19	112.36
3	L	1001	DEX	F1-C9-C10	-4.03	100.76	104.19
3	D	1001	DEX	C2-C3-C4	-4.01	113.04	117.13
3	D	1001	DEX	C19-C10-C9	3.90	116.34	113.55
3	H	1001	DEX	C7-C8-C9	-3.81	107.43	110.94
3	H	1001	DEX	C22-C16-C17	3.75	123.05	115.01
3	A	1001	DEX	C12-C13-C17	3.73	118.62	115.57
3	A	1001	DEX	F1-C9-C10	-3.67	101.07	104.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	DEX	C12-C11-C9	-3.62	110.39	112.93
3	D	1001	DEX	C12-C13-C14	-3.53	104.91	108.03
3	L	1001	DEX	C12-C13-C17	3.49	118.43	115.57
3	L	1001	DEX	C6-C5-C10	3.47	117.75	115.61
3	A	1001	DEX	C10-C1-C2	-3.38	121.92	124.38
3	L	1001	DEX	C22-C16-C17	3.36	122.23	115.01
3	L	1001	DEX	C18-C13-C17	-3.34	105.14	110.39
3	H	1001	DEX	C12-C13-C14	3.31	110.97	108.03
3	A	1001	DEX	C15-C14-C8	-3.29	116.02	119.07
3	H	1001	DEX	C15-C14-C8	-3.22	116.08	119.07
3	L	1001	DEX	C15-C14-C13	3.21	107.27	103.97
3	H	1001	DEX	C22-C16-C15	-3.17	108.43	113.53
3	D	1001	DEX	C10-C9-C8	3.02	116.05	112.12
3	L	1001	DEX	F1-C9-C8	-3.02	103.24	105.95
3	A	1001	DEX	C13-C14-C8	-2.97	111.39	113.73
3	L	1001	DEX	O3-C17-C13	-2.83	102.50	109.97
3	L	1001	DEX	C13-C14-C8	2.82	115.95	113.73
3	L	1001	DEX	C18-C13-C14	2.78	117.19	111.80
3	A	1001	DEX	C18-C13-C17	-2.71	106.14	110.39
3	A	1001	DEX	F1-C9-C11	-2.70	100.38	102.72
3	A	1001	DEX	F1-C9-C8	-2.69	103.53	105.95
3	L	1001	DEX	C10-C9-C8	2.66	115.58	112.12
3	A	1001	DEX	O3-C17-C20	2.64	113.06	107.04
3	L	1001	DEX	C19-C10-C1	-2.63	103.88	106.63
3	H	1001	DEX	C13-C17-C20	-2.57	110.16	112.89
3	A	1001	DEX	C7-C8-C14	-2.54	105.72	111.47
3	A	1001	DEX	C5-C4-C3	-2.54	120.50	122.72
3	L	1001	DEX	O5-C21-C20	-2.51	106.19	112.71
3	L	1001	DEX	O3-C17-C16	2.50	118.11	110.74
3	H	1001	DEX	C19-C10-C9	2.46	115.31	113.55
3	D	1001	DEX	C15-C14-C13	2.44	106.48	103.97
3	H	1001	DEX	C17-C13-C14	-2.41	97.10	99.36
3	L	1001	DEX	C12-C11-C9	2.37	114.58	112.93
3	A	1001	DEX	C13-C17-C16	2.27	105.01	102.86
3	L	1001	DEX	C13-C17-C16	2.23	104.97	102.86
3	H	1001	DEX	C7-C8-C14	-2.23	106.44	111.47
3	D	1001	DEX	C19-C10-C5	-2.22	105.02	107.76
3	H	1001	DEX	C10-C5-C4	-2.22	120.51	122.12
3	D	1001	DEX	C7-C8-C9	-2.20	108.91	110.94
3	A	1001	DEX	C1-C2-C3	-2.16	119.63	121.47
3	A	1001	DEX	O5-C21-C20	-2.14	107.15	112.71
3	D	1001	DEX	F1-C9-C11	2.09	104.54	102.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1001	DEX	C1-C10-C5	-2.09	111.25	112.36
3	D	1001	DEX	C12-C11-C9	-2.05	111.49	112.93
3	H	1001	DEX	C19-C10-C1	-2.05	104.48	106.63
3	A	1001	DEX	C19-C10-C1	-2.05	104.49	106.63
3	A	1001	DEX	C7-C6-C5	-2.03	108.10	111.93

There are no chirality outliers.

All (6) torsion outliers are listed below:

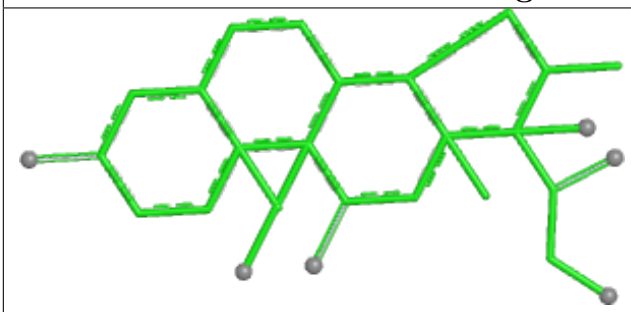
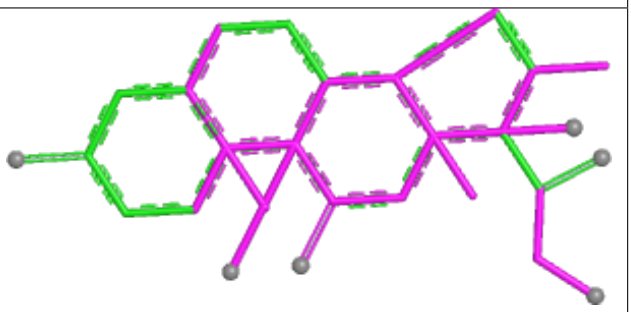
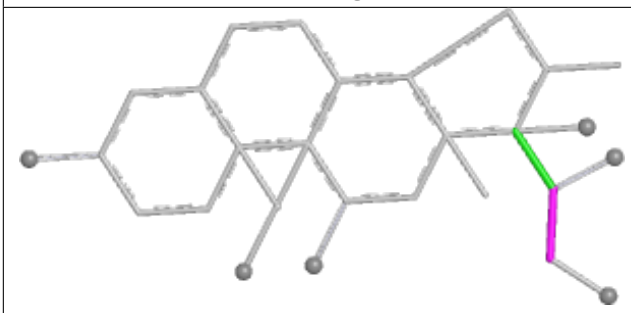
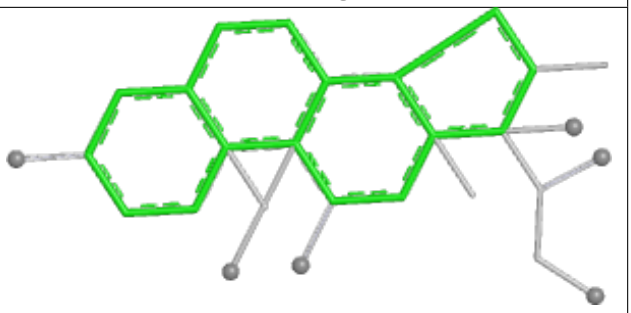
Mol	Chain	Res	Type	Atoms
3	D	1001	DEX	C17-C20-C21-O5
3	D	1001	DEX	O4-C20-C21-O5
3	A	1001	DEX	C17-C20-C21-O5
3	L	1001	DEX	C17-C20-C21-O5
3	A	1001	DEX	O4-C20-C21-O5
3	H	1001	DEX	O4-C20-C21-O5

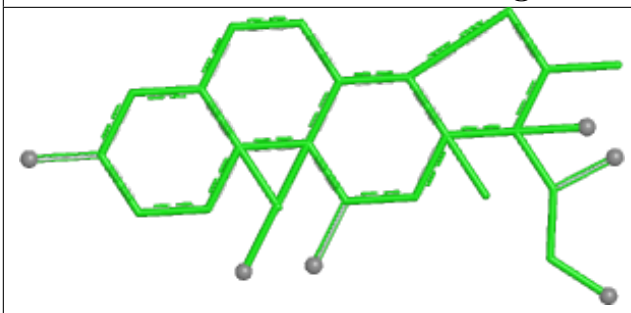
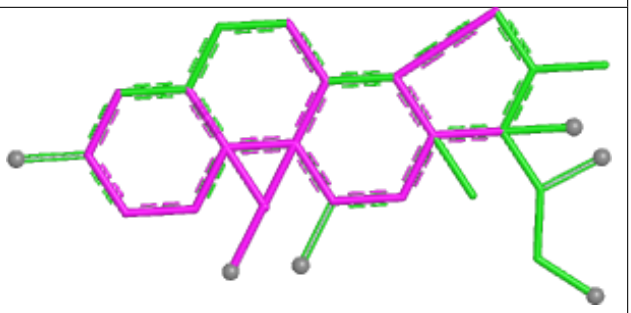
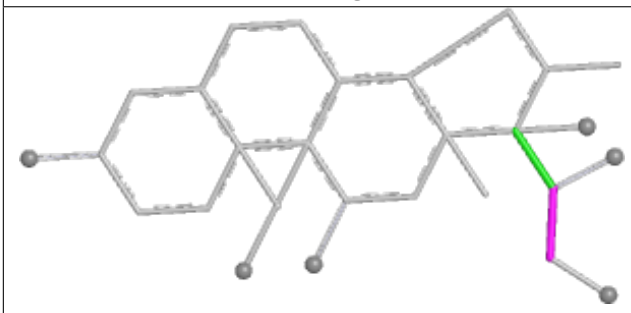
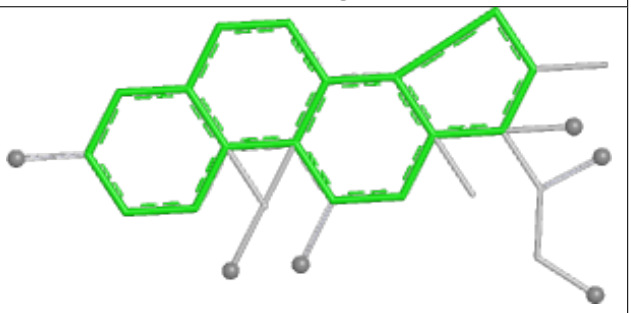
There are no ring outliers.

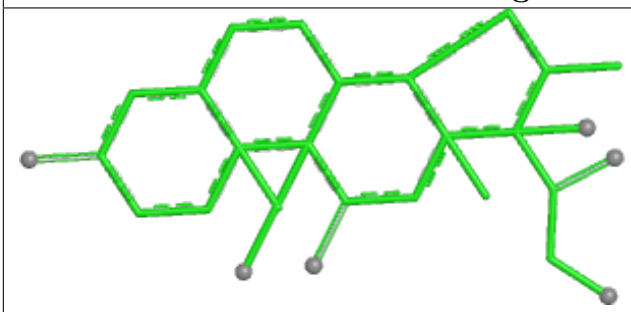
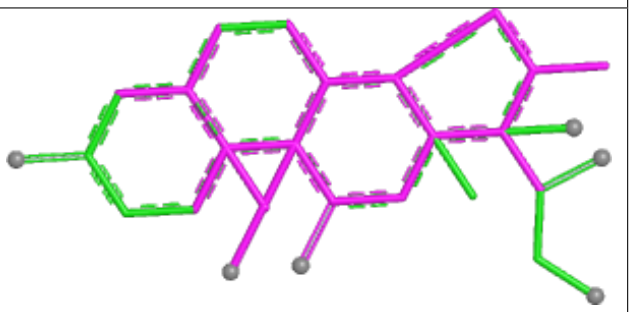
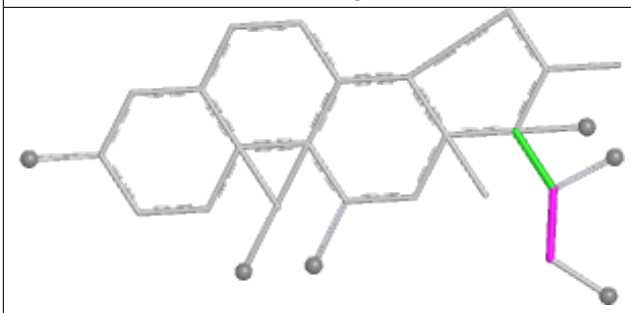
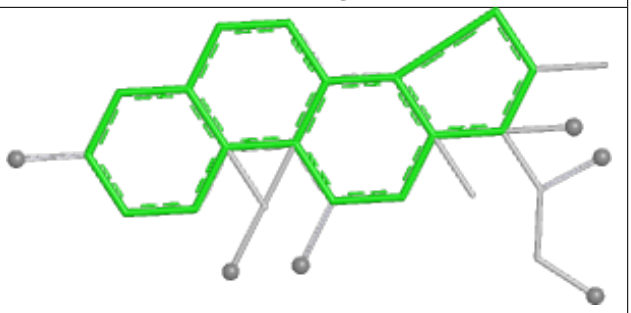
4 monomers are involved in 15 short contacts:

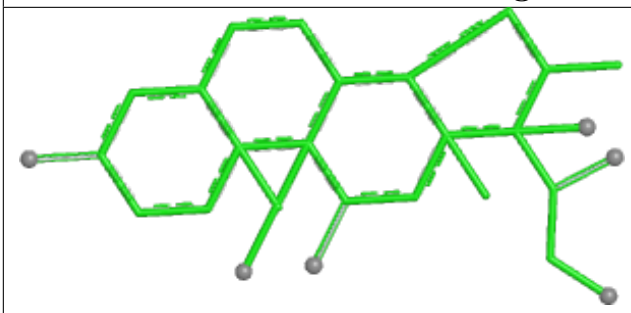
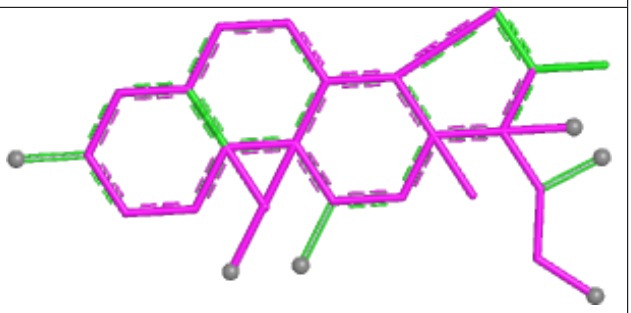
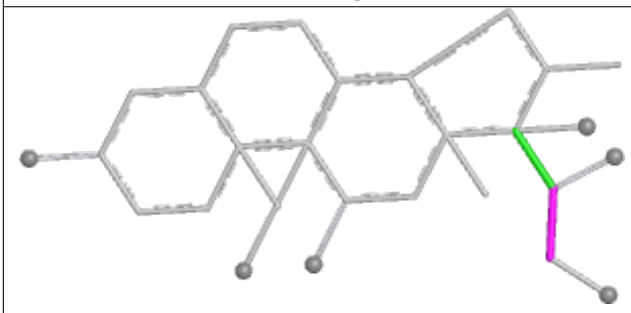
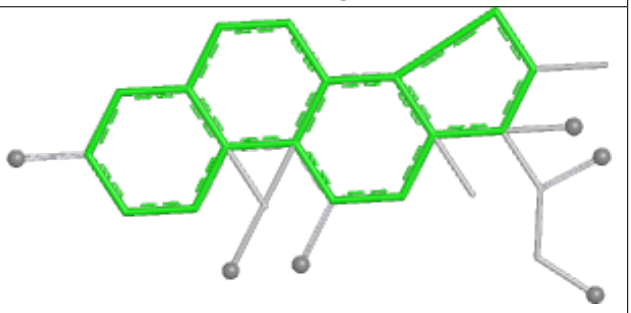
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1001	DEX	3	0
3	D	1001	DEX	3	0
3	H	1001	DEX	5	0
3	A	1001	DEX	4	0

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.

Ligand DEX L 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DEX D 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DEX H 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DEX A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	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	H	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	C	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	N	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	A	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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

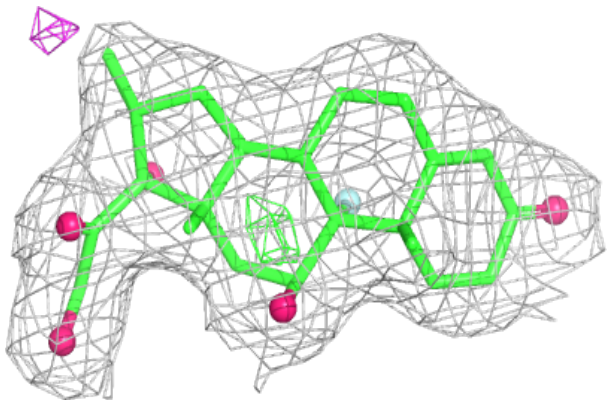
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

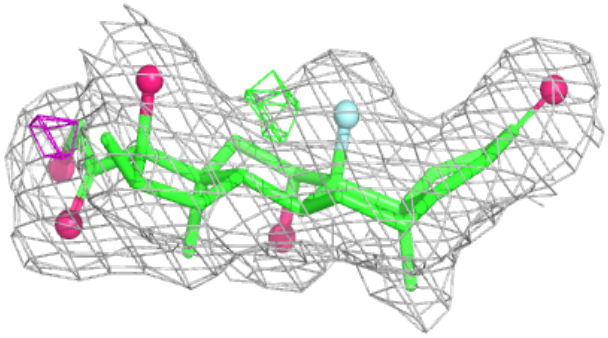
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DEX	A	1001	28/28	0.99	0.11	21,26,31,32	0
3	DEX	D	1001	28/28	0.99	0.11	21,29,37,40	0
3	DEX	H	1001	28/28	0.99	0.12	19,25,35,41	0
3	DEX	L	1001	28/28	0.99	0.12	19,26,34,45	0
4	NA	H	1002	1/1	1.00	0.11	23,23,23,23	0

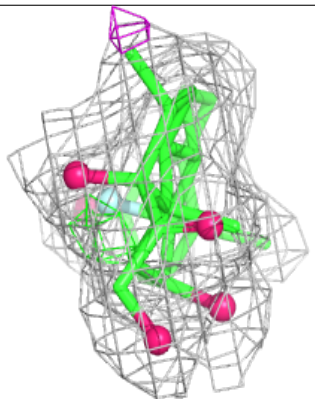
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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)

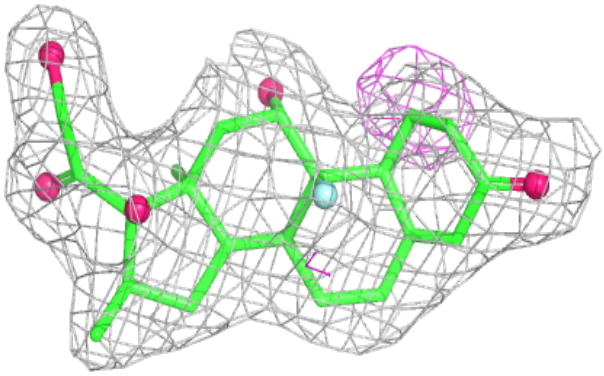


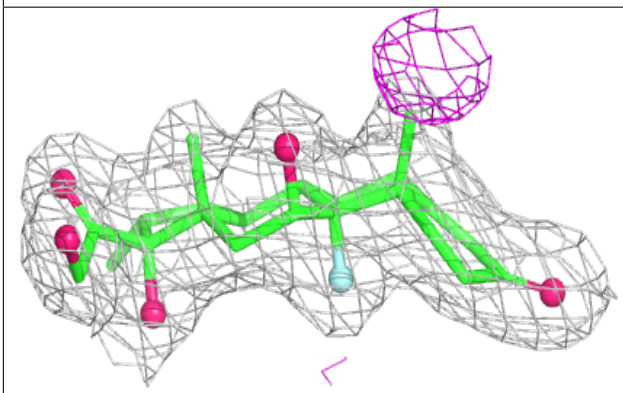


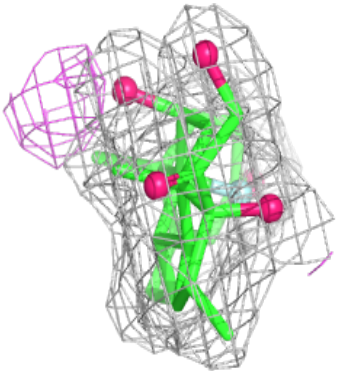


Electron density around DEX D 1001:

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

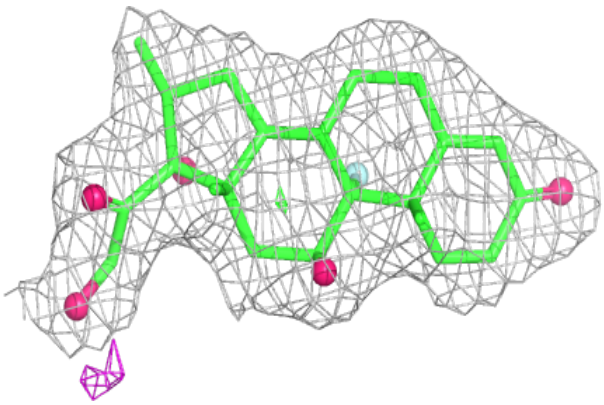


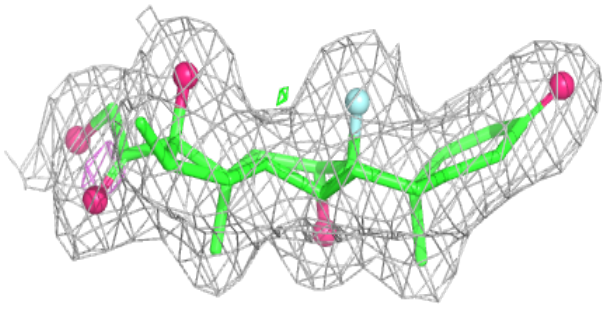


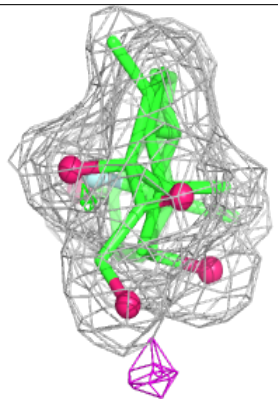


Electron density around DEX H 1001:

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

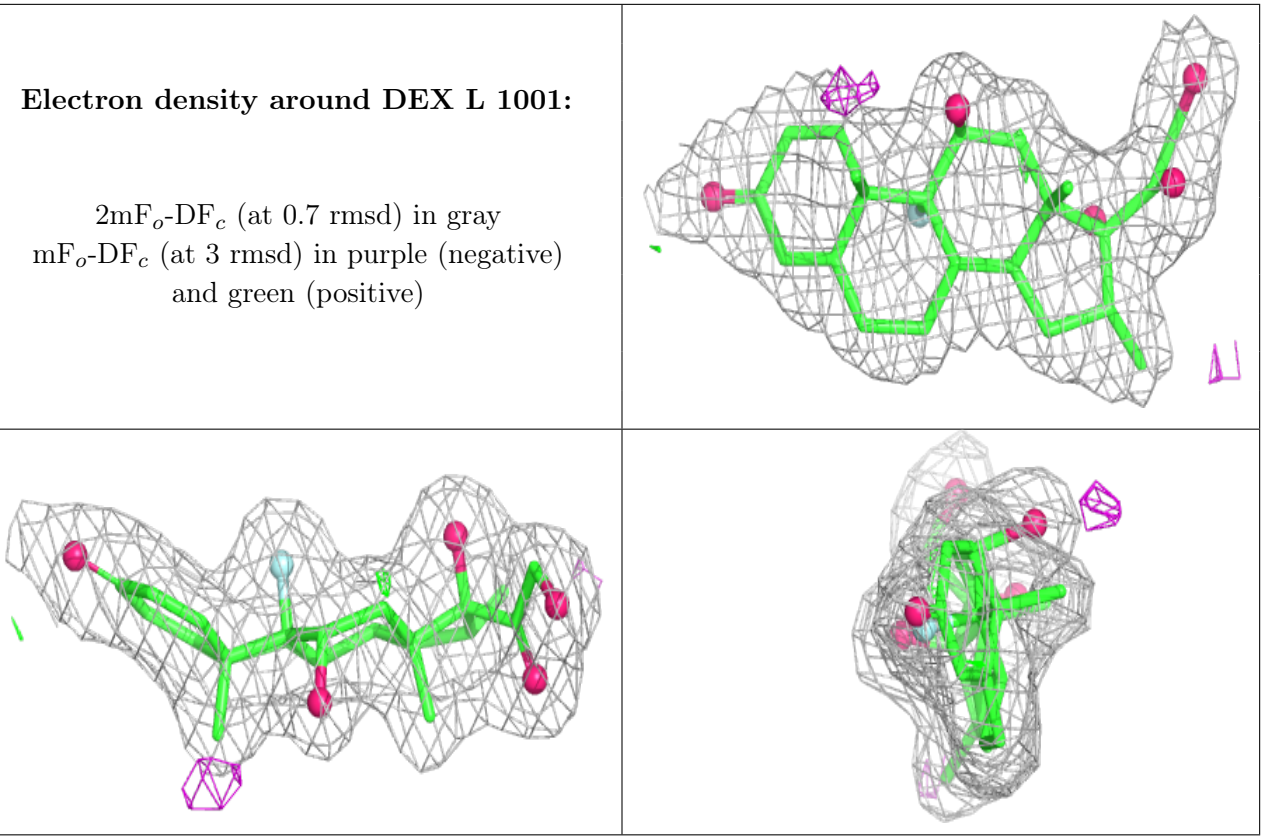






Electron density around DEX L 1001:

$2mF_o$-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.