Full wwPDB X-ray Structure Validation Report (i)

Nov 30, 2022 – 03:17 pm GMT

PDB ID	:	7YXO
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	:	2.99 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 (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 (i)) were used in the production of this report:

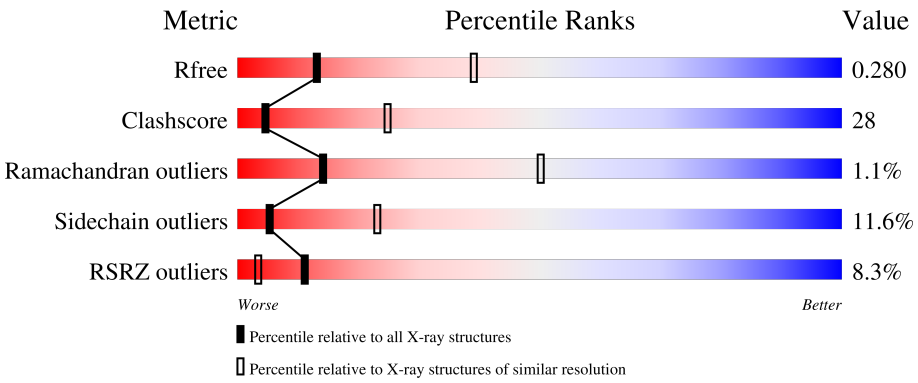
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	4% 57% 32% 6% •
1	C	248	6% 50% 40% 5% •
1	E	248	14% 43% 39% 10% • 7%
2	B	11	45% 45% 9%
2	D	11	18% 55% 9% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	11	27% 36% 18% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CPS	A	1002	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6109 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
			Total	C	N	O	S			
1	A	237	1922	1246	314	345	17	0	0	0
1	C	237	1924	1247	315	345	17	0	0	0
1	E	230	1860	1208	300	335	17	0	0	0

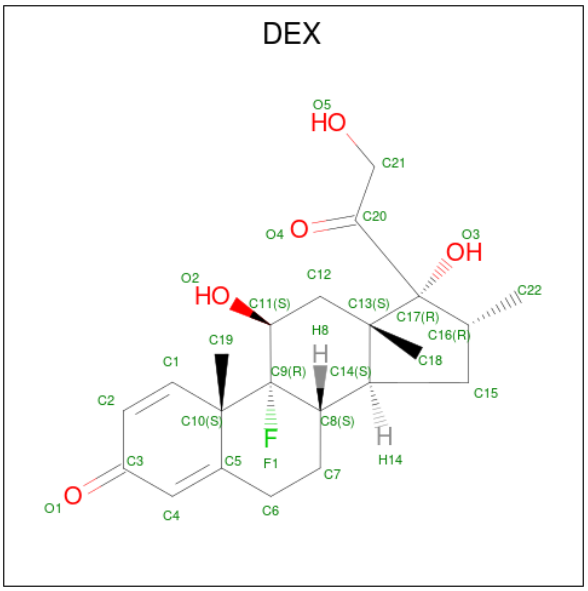
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	529	PHE	-	expression tag	UNP A0A1X8XLE9
C	529	PHE	-	expression tag	UNP A0A1X8XLE9
E	529	PHE	-	expression tag	UNP A0A1X8XLE9

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

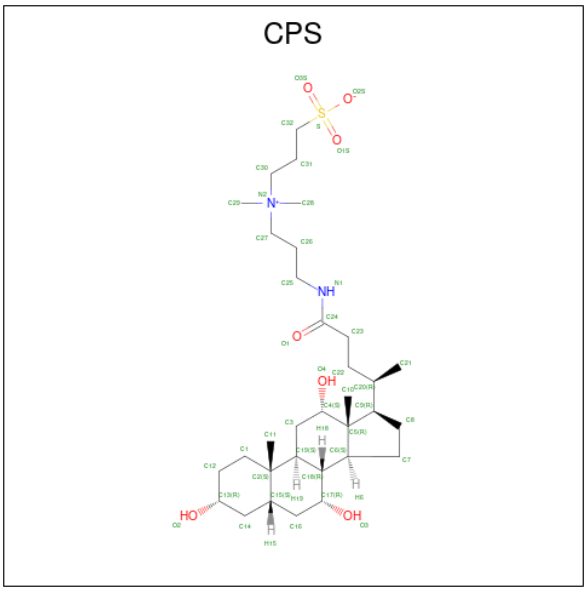
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	10	78	53	13	12	0	0	0
2	D	9	67	47	9	11	0	0	0
2	F	9	67	47	9	11	0	0	0

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



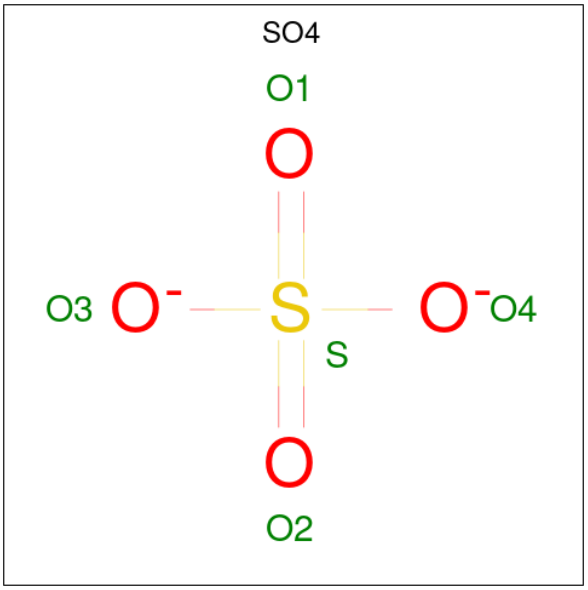
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
3	A	1	28	22	1	5	0	0
			Total	C	F	O		
3	C	1	28	22	1	5	0	0
			Total	C	F	O		
3	E	1	28	22	1	5	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	42	32	2	7	1	0	0
			Total	C	N	O	S		
4	C	1	42	32	2	7	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	C	1	5	4	1	0	0
			Total	O	S		
5	C	1	5	4	1	0	0

- Molecule 6 is water.

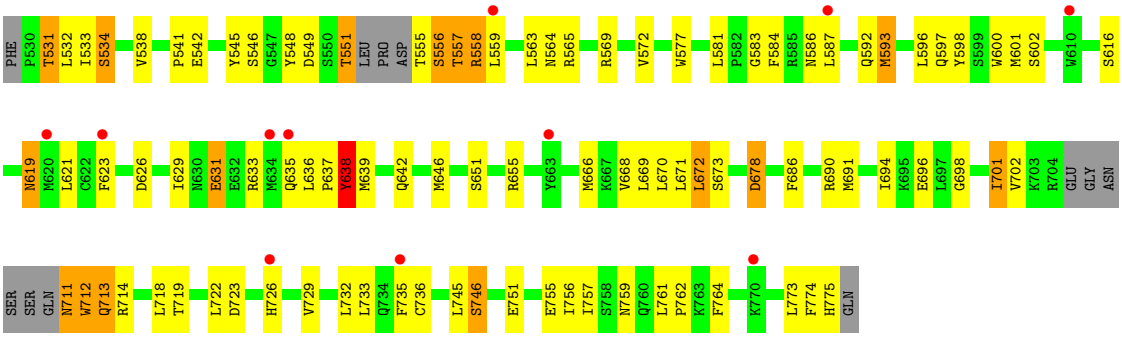
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	5	5	5	0	0
			Total	O		
6	C	2	2	2	0	0
			Total	O		
6	E	1	1	1	0	0

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.

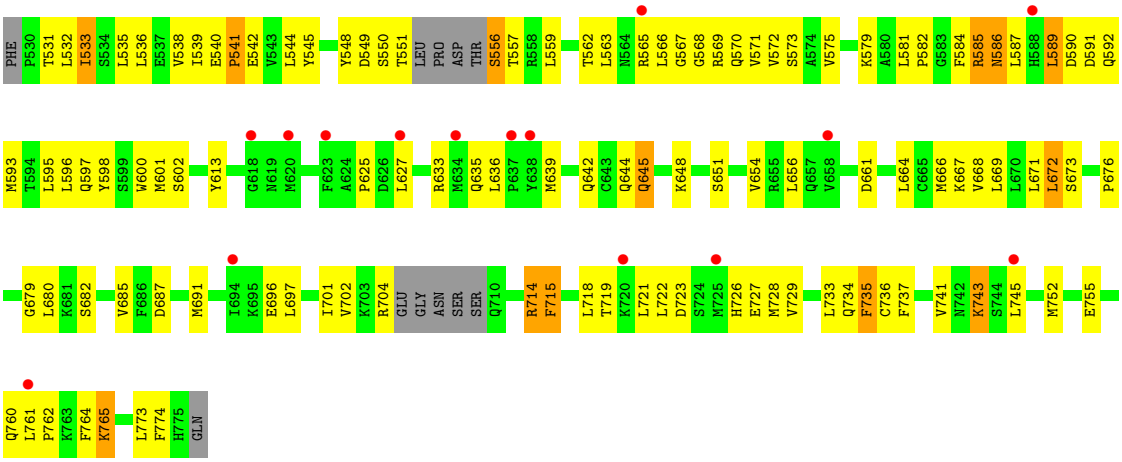
• Molecule 1: Ancestral Glucocorticoid Receptor2

Chain A:



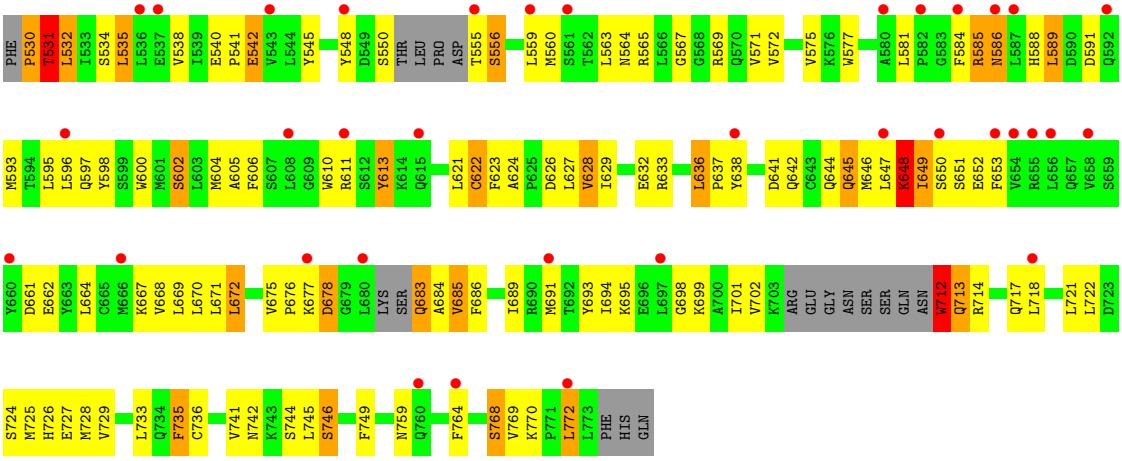
• Molecule 1: Ancestral Glucocorticoid Receptor2

Chain C:



• Molecule 1: Ancestral Glucocorticoid Receptor2

Chain E:

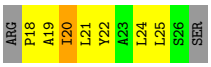


- Molecule 2: SHP NR Box 1 Peptide

Chain B:

- Molecule 2: SHP NR Box 1 Peptide

Chain D:



- Molecule 2: SHP NR Box 1 Peptide

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	180.20Å 180.20Å 169.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.10 – 2.99 90.10 – 3.18	Depositor EDS
% Data completeness (in resolution range)	83.5 (90.10-2.99) 83.5 (90.10-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.242 , 0.280 0.242 , 0.280	Depositor DCC
R_{free} test set	1194 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	73.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Reported twinning fraction	0.748 for H, K, L 0.124 for L, -K, H 0.128 for -H, L, K	Depositor
Outliers	0 of 23687 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CPS, SO4, 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	0.38	0/1962	0.84	3/2644 (0.1%)
1	C	0.37	0/1964	0.81	1/2646 (0.0%)
1	E	0.39	0/1897	0.88	7/2556 (0.3%)
2	B	0.49	0/79	1.00	0/107
2	D	0.45	0/68	0.67	0/92
2	F	0.44	0/68	0.91	0/92
All	All	0.38	0/6038	0.84	11/8137 (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	E	0	3
All	All	0	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	713	GLN	CB-CA-C	8.05	126.50	110.40
1	C	765	LYS	CB-CA-C	6.96	124.33	110.40
1	E	531	THR	N-CA-C	-6.92	92.32	111.00
1	E	648	LYS	CB-CA-C	5.91	122.22	110.40
1	A	619	ASN	CB-CA-C	5.87	122.13	110.40
1	E	712	TRP	N-CA-C	5.72	126.45	111.00
1	E	712	TRP	C-N-CA	5.36	135.10	121.70
1	E	712	TRP	O-C-N	-5.35	114.14	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	557	THR	CA-CB-OG1	-5.33	97.81	109.00
1	E	530	PRO	C-N-CA	5.17	134.63	121.70
1	E	530	PRO	CB-CA-C	-5.08	99.31	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	638	TYR	Peptide
1	A	711	ASN	Peptide
1	E	530	PRO	Peptide
1	E	531	THR	Mainchain
1	E	712	TRP	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	1922	0	1957	101	1
1	C	1924	0	1958	102	0
1	E	1860	0	1896	133	2
2	B	78	0	87	4	0
2	D	67	0	75	11	0
2	F	67	0	75	9	0
3	A	28	0	29	5	0
3	C	28	0	29	1	0
3	E	28	0	29	1	0
4	A	42	0	58	21	0
4	C	42	0	58	8	0
5	A	5	0	0	0	0
5	C	10	0	0	0	0
6	A	5	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
All	All	6109	0	6251	348	2

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 28.

All (348) 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:702:VAL:HG22	1:A:711:ASN:ND2	1.16	1.47
4:A:1002:CPS:H23	4:A:1002:CPS:C8	1.53	1.37
1:A:702:VAL:CG2	1:A:711:ASN:ND2	2.05	1.20
4:A:1002:CPS:H25	4:A:1002:CPS:H28B	1.27	1.16
4:C:1002:CPS:H10B	4:C:1002:CPS:H21A	1.18	1.15
4:A:1002:CPS:H8A	4:A:1002:CPS:C23	1.74	1.09
1:E:675:VAL:HG21	1:E:772:LEU:CD1	1.88	1.03
1:E:675:VAL:CG2	1:E:772:LEU:HD11	1.87	1.02
1:A:712:TRP:CZ2	4:A:1002:CPS:H21	1.97	0.99
4:A:1002:CPS:H28B	4:A:1002:CPS:C25	1.93	0.99
1:E:675:VAL:HG21	1:E:772:LEU:HD11	0.97	0.97
1:E:531:THR:O	1:E:531:THR:HG23	1.63	0.95
1:A:702:VAL:HG22	1:A:711:ASN:HD22	1.31	0.94
1:A:711:ASN:ND2	4:A:1002:CPS:H29B	1.84	0.92
1:E:532:LEU:HD22	1:E:532:LEU:H	1.36	0.91
4:C:1002:CPS:H21A	4:C:1002:CPS:C10	2.02	0.89
1:E:685:VAL:HG12	1:E:689:ILE:HD11	1.54	0.88
4:A:1002:CPS:C8	4:A:1002:CPS:C23	2.42	0.88
1:A:597:GLN:OE1	1:A:759:ASN:ND2	2.08	0.87
1:C:666:MET:HB3	1:C:722:LEU:HD21	1.58	0.85
1:E:652:GLU:HB3	1:E:721:LEU:HD21	1.60	0.83
1:C:639:MET:HA	1:C:642:GLN:HE21	1.42	0.82
1:E:698:GLY:O	1:E:702:VAL:HG23	1.80	0.82
1:A:636:LEU:HD22	1:C:648:LYS:HZ3	1.45	0.81
1:A:621:LEU:HB3	1:A:623:PHE:HE2	1.47	0.80
1:E:645:GLN:OE1	1:E:728:MET:HA	1.81	0.80
1:A:751:GLU:O	1:A:755:GLU:HG3	1.82	0.79
1:A:702:VAL:HG22	1:A:711:ASN:HD21	1.01	0.79
1:E:652:GLU:HG3	1:E:721:LEU:HD11	1.62	0.79
1:A:712:TRP:HZ2	4:A:1002:CPS:H21	1.41	0.79
1:A:639:MET:HA	1:A:642:GLN:HE21	1.45	0.79
1:A:636:LEU:HD22	1:C:648:LYS:NZ	1.97	0.79
2:D:21:LEU:O	2:D:25:LEU:HG	1.81	0.79
1:E:622:CYS:HA	1:E:627:LEU:O	1.83	0.79
1:E:683:GLN:O	1:E:686:PHE:HB3	1.85	0.77
4:A:1002:CPS:H23	4:A:1002:CPS:H8A	0.81	0.77
1:E:531:THR:O	1:E:531:THR:CG2	2.27	0.77
1:A:702:VAL:CG2	1:A:711:ASN:HD21	1.80	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:LEU:C	2:F:21:LEU:HD13	2.05	0.76
4:C:1002:CPS:H10B	4:C:1002:CPS:C21	2.06	0.76
1:C:736:CYS:HA	3:C:1001:DEX:O4	1.86	0.76
1:C:737:PHE:CD1	1:C:761:LEU:HD13	2.21	0.76
1:E:532:LEU:H	1:E:532:LEU:CD2	2.00	0.75
1:E:541:PRO:HD3	1:E:577:TRP:CD1	2.22	0.75
2:F:21:LEU:HD13	2:F:21:LEU:O	1.86	0.75
4:A:1002:CPS:H25	4:A:1002:CPS:C28	2.13	0.75
1:E:652:GLU:HB3	1:E:721:LEU:CD2	2.17	0.73
1:E:669:LEU:O	1:E:672:LEU:N	2.21	0.73
1:C:669:LEU:O	1:C:672:LEU:N	2.21	0.72
1:E:725:MET:O	1:E:728:MET:N	2.18	0.72
1:A:564:ASN:OD1	3:A:1001:DEX:H211	1.91	0.71
1:E:695:LYS:O	1:E:699:LYS:HG3	1.89	0.71
1:E:648:LYS:HE2	1:E:651:SER:OG	1.91	0.71
1:A:616:SER:O	1:A:619:ASN:HB3	1.91	0.71
1:A:669:LEU:O	1:A:672:LEU:N	2.23	0.70
4:A:1002:CPS:C25	4:A:1002:CPS:C28	2.69	0.70
1:C:589:LEU:CD1	1:C:593:MET:CE	2.70	0.69
1:E:559:LEU:O	1:E:563:LEU:HG	1.93	0.69
1:A:702:VAL:CG2	1:A:711:ASN:HD22	1.92	0.69
1:E:669:LEU:CD1	1:E:722:LEU:HD11	2.22	0.68
1:C:755:GLU:HB3	2:D:18:PRO:HB3	1.76	0.68
1:A:736:CYS:HA	3:A:1001:DEX:O4	1.93	0.68
1:E:602:SER:O	1:E:605:ALA:HB3	1.93	0.68
1:C:593:MET:SD	2:D:25:LEU:HD12	2.34	0.68
1:A:712:TRP:CE2	4:A:1002:CPS:H21	2.28	0.68
1:E:613:TYR:CD1	1:E:613:TYR:C	2.66	0.67
1:C:639:MET:HA	1:C:642:GLN:NE2	2.10	0.67
1:A:531:THR:HG23	1:A:534:SER:HB3	1.77	0.67
1:A:559:LEU:O	1:A:563:LEU:HG	1.95	0.66
1:A:678:ASP:N	1:A:678:ASP:OD1	2.26	0.66
1:A:691:MET:HA	1:A:694:ILE:HD12	1.78	0.66
1:E:678:ASP:OD1	1:E:678:ASP:N	2.28	0.66
1:A:621:LEU:HB3	1:A:623:PHE:CE2	2.28	0.66
1:E:532:LEU:HD22	1:E:532:LEU:N	2.09	0.66
1:C:687:ASP:HB2	4:C:1002:CPS:H28B	1.78	0.65
1:E:648:LYS:HA	1:E:651:SER:OG	1.97	0.65
1:E:669:LEU:CD1	1:E:722:LEU:CD1	2.75	0.65
1:E:713:GLN:O	1:E:717:GLN:HG3	1.96	0.65
1:E:691:MET:HA	1:E:694:ILE:HD12	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:LEU:HD22	3:A:1001:DEX:H511	1.77	0.65
1:A:701:ILE:HD11	1:A:718:LEU:HD12	1.78	0.64
1:C:549:ASP:HB3	1:C:551:THR:HB	1.79	0.64
1:C:639:MET:O	1:C:642:GLN:HG2	1.97	0.63
1:C:544:LEU:HD13	1:E:542:GLU:OE2	1.99	0.63
1:C:585:ARG:HH12	2:F:26:SER:HA	1.63	0.63
1:A:722:LEU:HD22	1:A:774:PHE:CE2	2.33	0.63
1:E:722:LEU:O	1:E:726:HIS:CE1	2.51	0.63
1:A:759:ASN:O	1:A:762:PRO:HD2	1.98	0.63
1:C:533:ILE:HG23	1:C:661:ASP:OD2	1.98	0.63
1:E:652:GLU:CB	1:E:721:LEU:HD21	2.28	0.63
1:E:669:LEU:HD12	1:E:722:LEU:CD1	2.29	0.63
1:E:669:LEU:HD13	1:E:722:LEU:HD11	1.80	0.62
1:A:712:TRP:HZ2	4:A:1002:CPS:C21	2.12	0.62
1:C:559:LEU:O	1:C:563:LEU:HG	1.99	0.62
1:A:541:PRO:HD3	1:A:577:TRP:CD1	2.34	0.61
1:C:572:VAL:HG11	1:E:538:VAL:O	1.99	0.61
1:C:645:GLN:OE1	1:C:728:MET:O	2.19	0.61
1:E:645:GLN:NE2	1:E:728:MET:HB3	2.15	0.61
1:C:589:LEU:CD1	1:C:593:MET:HE2	2.30	0.61
1:E:661:ASP:HA	1:E:664:LEU:HD12	1.83	0.61
1:C:714:ARG:HE	1:C:718:LEU:HD11	1.67	0.60
1:E:642:GLN:HB3	1:E:735:PHE:CE2	2.36	0.60
1:E:645:GLN:OE1	1:E:728:MET:CA	2.50	0.60
1:E:645:GLN:HE22	1:E:728:MET:HB3	1.67	0.60
1:C:545:TYR:CE1	1:E:545:TYR:CE1	2.90	0.60
1:C:682:SER:HB2	1:C:685:VAL:CG2	2.32	0.60
1:C:755:GLU:OE1	2:D:19:ALA:N	2.32	0.60
1:A:719:THR:HB	1:A:774:PHE:CD2	2.38	0.59
1:C:755:GLU:HG3	2:D:20:ILE:HD11	1.83	0.59
1:E:685:VAL:O	1:E:689:ILE:HG13	2.02	0.59
2:B:21:LEU:HD13	2:B:21:LEU:O	2.03	0.59
1:C:556:SER:OG	1:C:636:LEU:HB3	2.03	0.59
1:E:613:TYR:HD1	1:E:613:TYR:O	1.85	0.59
1:C:752:MET:HA	2:D:20:ILE:HD13	1.83	0.59
1:E:675:VAL:CG2	1:E:772:LEU:CD1	2.65	0.58
4:A:1002:CPS:H23	4:A:1002:CPS:H8	1.74	0.58
1:C:585:ARG:NH1	2:F:26:SER:HA	2.18	0.58
1:E:646:MET:HA	1:E:649:ILE:HD12	1.85	0.58
1:A:723:ASP:OD1	1:A:773:LEU:HA	2.04	0.58
1:C:532:LEU:HD13	1:C:536:LEU:HD13	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:560:MET:O	1:E:564:ASN:OD1	2.22	0.57
1:E:769:VAL:HG23	1:E:769:VAL:O	2.05	0.57
1:E:628:VAL:O	1:E:628:VAL:CG2	2.52	0.56
1:E:759:ASN:OD1	2:F:18:PRO:CD	2.53	0.56
1:C:687:ASP:CB	4:C:1002:CPS:H28B	2.35	0.56
1:A:722:LEU:HD22	1:A:774:PHE:HE2	1.70	0.56
1:A:555:THR:HG22	1:A:557:THR:H	1.70	0.56
1:C:533:ILE:HG13	1:C:696:GLU:OE2	2.05	0.56
1:C:591:ASP:OD2	1:C:680:LEU:HB3	2.06	0.56
1:A:601:MET:HG3	1:A:729:VAL:HG13	1.87	0.56
1:E:540:GLU:OE2	1:E:667:LYS:CE	2.54	0.56
1:A:671:LEU:HD12	1:A:671:LEU:O	2.06	0.56
1:C:719:THR:HB	1:C:774:PHE:CD2	2.40	0.56
1:C:723:ASP:OD1	1:C:773:LEU:HA	2.06	0.55
1:A:555:THR:HG21	1:C:727:GLU:OE2	2.06	0.55
1:E:652:GLU:HG3	1:E:721:LEU:CD1	2.34	0.55
1:C:596:LEU:O	1:C:600:TRP:HB3	2.06	0.55
1:A:596:LEU:O	1:A:600:TRP:HB3	2.06	0.55
1:A:639:MET:HA	1:A:642:GLN:NE2	2.19	0.55
1:C:633:ARG:O	1:C:636:LEU:HB2	2.07	0.55
1:A:673:SER:HB3	1:A:726:HIS:NE2	2.21	0.54
1:A:698:GLY:O	1:A:702:VAL:HG23	2.07	0.54
1:C:687:ASP:HB3	4:C:1002:CPS:H271	1.89	0.54
1:E:669:LEU:HD13	1:E:722:LEU:CD1	2.37	0.54
1:A:631:GLU:O	1:A:631:GLU:HG3	2.07	0.54
1:C:589:LEU:HD12	1:C:593:MET:CE	2.37	0.54
1:E:676:PRO:HA	1:E:768:SER:O	2.06	0.54
1:A:711:ASN:CG	4:A:1002:CPS:H29B	2.28	0.54
1:E:556:SER:OG	1:E:637:PRO:HG2	2.08	0.54
1:E:691:MET:HG3	1:E:695:LYS:NZ	2.22	0.54
1:A:581:LEU:HB2	1:A:584:PHE:HB2	1.90	0.53
1:E:683:GLN:O	1:E:686:PHE:CB	2.56	0.53
1:A:548:TYR:HE2	1:A:633:ARG:NH2	2.06	0.53
1:C:570:GLN:O	1:C:573:SER:HB2	2.09	0.53
1:A:633:ARG:O	1:A:636:LEU:HB2	2.09	0.53
1:E:548:TYR:CE2	1:E:550:SER:HA	2.44	0.53
2:B:20:ILE:O	2:B:21:LEU:C	2.47	0.53
1:C:589:LEU:CD1	1:C:593:MET:HE1	2.40	0.52
1:A:666:MET:HA	1:A:669:LEU:HD12	1.91	0.52
1:E:596:LEU:O	1:E:600:TRP:HB3	2.09	0.52
1:E:649:ILE:HG21	1:E:725:MET:SD	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:GLU:OE2	1:C:667:LYS:HE2	2.09	0.52
1:A:642:GLN:OE1	3:A:1001:DEX:H212	2.10	0.52
1:E:669:LEU:HD12	1:E:722:LEU:HD12	1.92	0.52
1:E:613:TYR:CD1	1:E:613:TYR:O	2.62	0.52
1:E:588:HIS:CD2	1:E:589:LEU:HG	2.46	0.51
1:C:549:ASP:HB3	1:C:551:THR:CB	2.40	0.51
1:E:622:CYS:CA	1:E:627:LEU:O	2.57	0.51
1:A:761:LEU:C	1:A:761:LEU:HD23	2.31	0.51
1:E:593:MET:O	1:E:597:GLN:HB2	2.11	0.51
1:C:544:LEU:HD22	1:E:542:GLU:CB	2.41	0.51
1:C:755:GLU:OE1	2:D:18:PRO:HA	2.11	0.51
1:E:621:LEU:O	1:E:629:ILE:HB	2.11	0.51
1:C:532:LEU:HD12	1:C:696:GLU:HG2	1.93	0.50
1:A:556:SER:OG	1:A:637:PRO:O	2.28	0.50
2:B:21:LEU:HD13	2:B:21:LEU:C	2.31	0.50
1:C:566:LEU:HA	1:C:569:ARG:NH1	2.27	0.50
1:C:697:LEU:O	1:C:701:ILE:HG13	2.12	0.50
1:E:531:THR:CG2	1:E:534:SER:HB2	2.42	0.50
1:E:671:LEU:O	1:E:671:LEU:HD12	2.12	0.50
1:A:638:TYR:CE1	1:C:645:GLN:HG3	2.47	0.50
1:A:714:ARG:HE	1:A:718:LEU:HD11	1.77	0.50
1:C:581:LEU:HD13	1:C:668:VAL:HG13	1.94	0.50
1:E:569:ARG:O	1:E:572:VAL:HB	2.12	0.49
1:C:656:LEU:O	1:C:714:ARG:NH2	2.43	0.49
1:E:647:LEU:HA	1:E:650:SER:HB3	1.94	0.49
1:E:628:VAL:O	1:E:628:VAL:HG23	2.12	0.49
1:E:586:ASN:OD1	1:E:586:ASN:N	2.42	0.48
1:C:569:ARG:O	1:C:572:VAL:HB	2.13	0.48
1:A:563:LEU:HB3	3:A:1001:DEX:H11	1.94	0.48
1:E:724:SER:O	1:E:727:GLU:HG2	2.13	0.48
1:C:545:TYR:OH	1:C:625:PRO:HB2	2.13	0.48
1:E:610:TRP:CD1	1:E:610:TRP:C	2.86	0.48
1:C:671:LEU:O	1:C:671:LEU:HD12	2.13	0.48
1:A:761:LEU:C	1:A:761:LEU:CD2	2.82	0.48
1:E:624:ALA:HB3	1:E:626:ASP:OD1	2.14	0.47
1:E:649:ILE:O	1:E:653:PHE:CD2	2.67	0.47
1:A:598:TYR:N	1:A:598:TYR:CD2	2.83	0.47
1:A:691:MET:SD	4:A:1002:CPS:O2	2.69	0.47
1:A:712:TRP:NE1	4:A:1002:CPS:H21	2.28	0.47
1:A:686:PHE:HE1	1:A:690:ARG:HD2	1.79	0.47
1:A:712:TRP:CD1	4:A:1002:CPS:H25A	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:LEU:HD13	1:C:593:MET:HE2	1.97	0.47
1:E:540:GLU:OE2	1:E:667:LYS:NZ	2.47	0.47
1:E:662:GLU:OE2	1:E:701:ILE:HG12	2.15	0.47
1:E:535:LEU:O	1:E:538:VAL:HG22	2.15	0.47
1:C:535:LEU:O	1:C:538:VAL:HG22	2.15	0.47
1:C:682:SER:HB2	1:C:685:VAL:HG21	1.97	0.47
1:C:587:LEU:O	1:C:592:GLN:NE2	2.48	0.46
1:A:533:ILE:HG13	1:A:696:GLU:OE2	2.15	0.46
1:A:569:ARG:O	1:A:572:VAL:HB	2.14	0.46
1:C:584:PHE:CE1	1:C:671:LEU:HD21	2.50	0.46
1:A:546:SER:OG	1:A:626:ASP:OD1	2.33	0.46
1:C:735:PHE:HD1	1:C:735:PHE:O	1.97	0.46
1:A:581:LEU:HB2	1:A:584:PHE:CB	2.46	0.46
1:C:702:VAL:C	1:C:704:ARG:H	2.19	0.46
1:E:613:TYR:CD2	1:E:653:PHE:HB3	2.51	0.46
2:D:20:ILE:H	2:D:20:ILE:HG13	1.36	0.46
1:C:635:GLN:HA	1:C:635:GLN:OE1	2.16	0.46
1:C:597:GLN:HG2	1:C:760:GLN:HB2	1.98	0.46
1:C:644:GLN:OE1	1:C:644:GLN:HA	2.16	0.46
1:A:646:MET:HG2	1:A:732:LEU:HD11	1.97	0.46
1:E:595:LEU:HD21	1:E:675:VAL:HG12	1.98	0.46
1:A:666:MET:HE2	1:A:718:LEU:HD13	1.98	0.45
1:E:532:LEU:HD13	1:E:535:LEU:HD13	1.98	0.45
1:E:668:VAL:HG11	1:E:693:TYR:CE1	2.51	0.45
1:A:636:LEU:O	1:A:639:MET:HB2	2.15	0.45
1:A:638:TYR:HE1	1:C:645:GLN:HG3	1.78	0.45
1:C:539:ILE:CG2	2:F:24:LEU:CD2	2.94	0.45
1:A:531:THR:HG23	1:A:534:SER:CB	2.43	0.45
1:A:601:MET:HG2	1:A:733:LEU:HG	1.99	0.45
1:A:666:MET:O	1:A:669:LEU:HB2	2.17	0.45
1:E:564:ASN:ND2	1:E:749:PHE:CE1	2.84	0.45
1:E:649:ILE:CG2	1:E:725:MET:SD	3.04	0.45
1:E:741:VAL:HG23	1:E:742:ASN:OD1	2.16	0.45
1:A:598:TYR:N	1:A:598:TYR:HD2	2.13	0.45
1:A:761:LEU:HD23	1:A:761:LEU:O	2.16	0.45
1:E:613:TYR:C	1:E:613:TYR:HD1	2.17	0.45
1:E:759:ASN:OD1	2:F:18:PRO:HD3	2.16	0.45
1:A:774:PHE:C	1:A:775:HIS:ND1	2.70	0.45
1:C:601:MET:HG3	1:C:729:VAL:HG13	1.99	0.45
1:C:651:SER:O	1:C:654:VAL:HB	2.17	0.45
1:E:598:TYR:N	1:E:598:TYR:CD2	2.83	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ILE:O	1:A:761:LEU:HB2	2.17	0.45
1:C:575:VAL:O	1:C:579:LYS:HG3	2.17	0.45
1:E:585:ARG:O	1:E:585:ARG:HG2	2.17	0.45
1:E:644:GLN:HA	1:E:644:GLN:OE1	2.16	0.45
1:C:593:MET:CE	2:D:25:LEU:HD12	2.47	0.44
1:C:598:TYR:HD2	1:C:598:TYR:N	2.16	0.44
1:A:587:LEU:O	1:A:592:GLN:NE2	2.50	0.44
1:C:682:SER:HB2	1:C:685:VAL:HG23	1.98	0.44
1:C:532:LEU:HD21	1:C:582:PRO:HG2	1.98	0.44
1:C:533:ILE:CG2	1:C:661:ASP:OD2	2.64	0.44
1:C:571:VAL:O	1:C:575:VAL:HG23	2.17	0.44
1:C:598:TYR:N	1:C:598:TYR:CD2	2.84	0.44
1:E:567:GLY:O	1:E:571:VAL:HG23	2.17	0.44
1:A:597:GLN:HG3	1:A:756:ILE:HG23	1.98	0.44
1:E:584:PHE:CE1	1:E:671:LEU:HD21	2.53	0.44
1:A:633:ARG:HA	1:A:636:LEU:HG	1.99	0.44
1:A:761:LEU:HB3	1:A:762:PRO:CD	2.47	0.44
1:C:761:LEU:N	1:C:762:PRO:HD2	2.33	0.44
1:A:583:GLY:O	1:A:586:ASN:HB2	2.17	0.44
1:E:675:VAL:HG22	1:E:770:LYS:O	2.17	0.44
1:A:712:TRP:CZ2	4:A:1002:CPS:C21	2.85	0.43
1:A:745:LEU:O	1:A:746:SER:C	2.56	0.43
1:C:540:GLU:HA	1:C:541:PRO:HD2	1.83	0.43
1:E:606:PHE:HB2	1:E:670:LEU:HD13	2.00	0.43
1:C:538:VAL:O	1:E:572:VAL:HG11	2.18	0.43
1:E:598:TYR:N	1:E:598:TYR:HD2	2.16	0.43
1:A:549:ASP:C	1:A:551:THR:H	2.21	0.43
1:C:656:LEU:HD12	1:C:721:LEU:HD22	2.00	0.43
1:C:666:MET:CB	1:C:722:LEU:HD21	2.40	0.43
1:E:604:MET:HB3	3:E:1001:DEX:H921	2.01	0.43
1:E:636:LEU:HD22	1:E:636:LEU:HA	1.88	0.43
1:A:532:LEU:HB3	1:A:696:GLU:OE2	2.19	0.43
1:A:593:MET:SD	2:B:22:TYR:HD1	2.41	0.43
4:C:1002:CPS:H31A	4:C:1002:CPS:H261	2.00	0.43
1:E:649:ILE:O	1:E:653:PHE:HD2	2.01	0.43
1:E:733:LEU:HD23	1:E:764:PHE:CE2	2.53	0.43
1:C:664:LEU:O	1:C:668:VAL:HG23	2.19	0.43
1:E:745:LEU:O	1:E:746:SER:C	2.57	0.43
1:E:571:VAL:O	1:E:575:VAL:HG23	2.19	0.43
2:F:25:LEU:H	2:F:25:LEU:HG	1.65	0.43
1:C:548:TYR:CD1	1:C:562:THR:HG21	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:LEU:O	2:D:21:LEU:HG	2.19	0.43
1:E:691:MET:HG3	1:E:695:LYS:HZ3	1.82	0.43
1:E:735:PHE:O	1:E:735:PHE:HD1	2.02	0.43
2:F:22:TYR:O	2:F:24:LEU:N	2.51	0.43
1:C:733:LEU:O	1:C:736:CYS:HB3	2.19	0.42
1:E:725:MET:O	1:E:729:VAL:N	2.51	0.42
1:A:711:ASN:ND2	4:A:1002:CPS:C29	2.70	0.42
1:C:733:LEU:HD23	1:C:764:PHE:CE2	2.54	0.42
1:A:636:LEU:CD2	1:C:648:LYS:HZ3	2.25	0.42
1:C:676:PRO:HB2	1:C:679:GLY:O	2.19	0.42
1:E:722:LEU:O	1:E:726:HIS:HE1	2.01	0.42
1:C:676:PRO:HD2	1:C:680:LEU:HD23	2.02	0.42
1:A:593:MET:O	1:A:597:GLN:HB2	2.19	0.42
1:C:595:LEU:HA	1:C:595:LEU:HD23	1.82	0.42
1:C:733:LEU:HD23	1:C:764:PHE:HE2	1.84	0.42
1:C:743:LYS:H	1:C:743:LYS:HG2	1.53	0.42
1:E:683:GLN:O	1:E:686:PHE:N	2.48	0.42
1:E:725:MET:C	1:E:728:MET:H	2.18	0.42
1:E:581:LEU:CB	1:E:584:PHE:HB2	2.48	0.42
1:E:606:PHE:CG	1:E:670:LEU:HD11	2.55	0.42
1:A:548:TYR:HE2	1:A:633:ARG:HH22	1.68	0.42
1:E:581:LEU:HB2	1:E:584:PHE:HB2	2.02	0.42
1:E:629:ILE:HG23	1:E:633:ARG:HB3	2.02	0.42
1:E:667:LYS:HA	1:E:670:LEU:HD12	2.02	0.42
1:C:666:MET:O	1:C:669:LEU:HB2	2.19	0.42
1:C:715:PHE:HE1	4:C:1002:CPS:HO2	1.68	0.42
1:E:713:GLN:O	1:E:717:GLN:CG	2.66	0.42
1:E:714:ARG:HH21	1:E:718:LEU:HD11	1.84	0.42
1:A:631:GLU:O	1:A:635:GLN:HG2	2.20	0.41
1:E:645:GLN:OE1	1:E:728:MET:CB	2.67	0.41
1:C:567:GLY:O	1:C:571:VAL:HG23	2.20	0.41
1:C:589:LEU:HD11	1:C:593:MET:HE1	2.01	0.41
1:E:671:LEU:HG	1:E:672:LEU:HD23	2.02	0.41
1:A:584:PHE:CE1	1:A:671:LEU:HD21	2.55	0.41
1:E:684:ALA:O	1:E:685:VAL:C	2.58	0.41
1:A:668:VAL:O	1:A:671:LEU:HB3	2.20	0.41
1:A:559:LEU:HD12	1:A:559:LEU:HA	1.96	0.41
1:A:733:LEU:HD23	1:A:733:LEU:HA	1.96	0.41
4:A:1002:CPS:H14	4:A:1002:CPS:H19	1.79	0.41
1:C:586:ASN:OD1	1:C:586:ASN:N	2.53	0.41
1:E:722:LEU:O	1:E:722:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:733:LEU:O	1:E:736:CYS:HB3	2.20	0.41
1:E:622:CYS:HB3	1:E:627:LEU:O	2.21	0.41
1:A:636:LEU:HA	1:A:637:PRO:HD2	1.65	0.41
1:C:589:LEU:HD21	2:D:25:LEU:O	2.21	0.41
1:E:595:LEU:HD23	1:E:595:LEU:HA	1.85	0.41
1:E:652:GLU:HB3	1:E:721:LEU:HD22	2.02	0.41
1:A:581:LEU:CB	1:A:584:PHE:HB2	2.50	0.41
1:A:745:LEU:HD11	1:C:734:GLN:HG2	2.02	0.41
1:C:633:ARG:HA	1:C:636:LEU:HG	2.03	0.41
1:C:673:SER:HB3	1:C:726:HIS:NE2	2.36	0.41
1:E:677:LYS:HG2	1:E:770:LYS:HB2	2.03	0.41
1:E:733:LEU:HD23	1:E:764:PHE:HE2	1.85	0.41
1:E:595:LEU:HD13	1:E:671:LEU:O	2.20	0.41
1:E:649:ILE:H	1:E:649:ILE:HG13	1.68	0.41
1:E:721:LEU:HD12	1:E:721:LEU:HA	1.88	0.41
1:A:621:LEU:HB2	1:A:629:ILE:HB	2.03	0.40
1:A:669:LEU:O	1:A:670:LEU:C	2.59	0.40
1:C:568:GLY:O	1:C:572:VAL:HG23	2.22	0.40
1:A:545:TYR:O	1:A:569:ARG:NH2	2.54	0.40
1:E:668:VAL:O	1:E:671:LEU:HB3	2.21	0.40
1:A:548:TYR:HE1	1:A:558:ARG:HD2	1.86	0.40
1:E:611:ARG:HH21	1:E:623:PHE:HA	1.86	0.40
1:E:652:GLU:HA	1:E:652:GLU:OE1	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:PHE:O	1:E:744:SER:OG[11_554]	1.93	0.27
1:E:712:TRP:CZ3	1:E:712:TRP:CZ3[6_556]	2.13	0.07

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	231/248 (93%)	209 (90%)	21 (9%)	1 (0%)	34	72
1	C	231/248 (93%)	207 (90%)	22 (10%)	2 (1%)	17	55
1	E	222/248 (90%)	197 (89%)	20 (9%)	5 (2%)	6	30
2	B	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
2	D	7/11 (64%)	7 (100%)	0	0	100	100
2	F	7/11 (64%)	4 (57%)	3 (43%)	0	100	100
All	All	706/777 (91%)	631 (89%)	67 (10%)	8 (1%)	14	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	685	VAL
1	E	713	GLN
1	E	532	LEU
1	C	541	PRO
1	E	531	THR
1	E	589	LEU
1	A	638	TYR
1	C	550	SER

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	217/227 (96%)	197 (91%)	20 (9%)	9	34
1	C	217/227 (96%)	194 (89%)	23 (11%)	6	26
1	E	210/227 (92%)	183 (87%)	27 (13%)	4	19
2	B	8/9 (89%)	6 (75%)	2 (25%)	0	3
2	D	7/9 (78%)	4 (57%)	3 (43%)	0	0
2	F	7/9 (78%)	5 (71%)	2 (29%)	0	2
All	All	666/708 (94%)	589 (88%)	77 (12%)	5	23

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	531	THR
1	A	534	SER
1	A	538	VAL
1	A	542	GLU
1	A	551	THR
1	A	556	SER
1	A	558	ARG
1	A	565	ARG
1	A	593	MET
1	A	602	SER
1	A	631	GLU
1	A	651	SER
1	A	655	ARG
1	A	672	LEU
1	A	678	ASP
1	A	701	ILE
1	A	712	TRP
1	A	713	GLN
1	A	735	PHE
1	A	746	SER
2	B	17	ARG
2	B	24	LEU
1	C	531	THR
1	C	533	ILE
1	C	542	GLU
1	C	556	SER
1	C	557	THR
1	C	565	ARG
1	C	585	ARG
1	C	586	ASN
1	C	589	LEU
1	C	590	ASP
1	C	602	SER
1	C	613	TYR
1	C	627	LEU
1	C	645	GLN
1	C	672	LEU
1	C	691	MET
1	C	714	ARG
1	C	715	PHE
1	C	735	PHE
1	C	741	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	743	LYS
1	C	745	LEU
1	C	765	LYS
2	D	20	ILE
2	D	22	TYR
2	D	24	LEU
1	E	535	LEU
1	E	542	GLU
1	E	555	THR
1	E	556	SER
1	E	565	ARG
1	E	585	ARG
1	E	586	ASN
1	E	591	ASP
1	E	602	SER
1	E	613	TYR
1	E	622	CYS
1	E	628	VAL
1	E	632	GLU
1	E	636	LEU
1	E	638	TYR
1	E	641	ASP
1	E	645	GLN
1	E	648	LYS
1	E	649	ILE
1	E	672	LEU
1	E	678	ASP
1	E	683	GLN
1	E	712	TRP
1	E	735	PHE
1	E	746	SER
1	E	768	SER
1	E	772	LEU
2	F	21	LEU
2	F	25	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	711	ASN
1	A	742	ASN
1	C	642	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	734	GLN
1	E	642	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)

8 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	A	1001	-	31,31,31	0.50	0	52,53,53	1.32	6 (11%)
5	SO4	C	1004	-	4,4,4	0.31	0	6,6,6	0.07	0
5	SO4	C	1003	-	4,4,4	0.36	0	6,6,6	0.13	0
4	CPS	A	1002	-	45,45,45	0.47	0	69,70,70	1.43	8 (11%)
4	CPS	C	1002	-	45,45,45	0.47	0	69,70,70	0.78	0
3	DEX	C	1001	-	31,31,31	0.49	0	52,53,53	1.17	4 (7%)
3	DEX	E	1001	-	31,31,31	0.40	0	52,53,53	1.51	10 (19%)
5	SO4	A	1003	-	4,4,4	0.37	0	6,6,6	0.06	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	A	1001	-	-	2/8/84/84	0/4/4/4
4	CPS	A	1002	-	-	17/25/90/90	0/4/4/4
4	CPS	C	1002	-	-	12/25/90/90	0/4/4/4
3	DEX	C	1001	-	-	2/8/84/84	0/4/4/4
3	DEX	E	1001	-	-	2/8/84/84	0/4/4/4

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1002	CPS	C15-C16-C17	6.02	121.10	114.46
3	A	1001	DEX	C6-C5-C10	4.63	118.46	115.61
3	E	1001	DEX	C9-C8-C14	3.70	112.13	109.26
3	E	1001	DEX	C13-C14-C8	3.66	116.61	113.73
4	A	1002	CPS	C9-C5-C6	-3.56	96.50	100.09
3	C	1001	DEX	C13-C17-C20	-3.55	109.13	112.89
4	A	1002	CPS	C16-C17-C18	3.46	115.18	111.48
4	A	1002	CPS	C19-C2-C15	-3.36	103.86	108.58
3	E	1001	DEX	C5-C4-C3	-3.21	119.91	122.72
3	C	1001	DEX	F1-C9-C11	-3.11	100.02	102.72
3	E	1001	DEX	F1-C9-C11	-3.07	100.06	102.72
3	A	1001	DEX	C13-C14-C8	-2.90	111.45	113.73
3	E	1001	DEX	C10-C9-C11	2.82	117.58	115.52
4	A	1002	CPS	C8-C9-C20	2.73	116.36	112.15
3	C	1001	DEX	C10-C9-C11	2.69	117.48	115.52
3	E	1001	DEX	C17-C13-C14	-2.66	96.87	99.36
3	E	1001	DEX	C10-C9-C8	-2.65	108.67	112.12
3	A	1001	DEX	C13-C17-C16	2.44	105.17	102.86
3	A	1001	DEX	C12-C13-C14	-2.33	105.97	108.03
3	E	1001	DEX	F1-C9-C8	2.31	108.02	105.95
3	A	1001	DEX	C15-C14-C8	-2.25	116.98	119.07
3	A	1001	DEX	C9-C8-C14	2.21	110.97	109.26
3	E	1001	DEX	C12-C13-C17	2.17	117.35	115.57
3	E	1001	DEX	C19-C10-C9	2.16	115.10	113.55
3	C	1001	DEX	C13-C17-C16	2.11	104.86	102.86
4	A	1002	CPS	C10-C5-C6	2.11	114.51	111.21
4	A	1002	CPS	C1-C12-C13	2.10	113.16	110.47
4	A	1002	CPS	C22-C23-C24	2.04	117.60	113.04

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	DEX	C17-C20-C21-O5
3	A	1001	DEX	O4-C20-C21-O5
3	C	1001	DEX	C17-C20-C21-O5
4	A	1002	CPS	C9-C20-C22-C23
4	A	1002	CPS	C25-C26-C27-N2
4	A	1002	CPS	C31-C30-N2-C27
4	A	1002	CPS	C31-C30-N2-C28
4	A	1002	CPS	C31-C32-S-O1S
4	A	1002	CPS	C21-C20-C9-C8
4	A	1002	CPS	C21-C20-C9-C5
4	C	1002	CPS	C26-C27-N2-C28
4	C	1002	CPS	C26-C27-N2-C29
4	C	1002	CPS	C21-C20-C9-C5
4	A	1002	CPS	C22-C20-C9-C5
4	C	1002	CPS	C26-C27-N2-C30
4	A	1002	CPS	C31-C32-S-O2S
4	A	1002	CPS	C22-C20-C9-C8
4	A	1002	CPS	C31-C30-N2-C29
4	A	1002	CPS	C22-C23-C24-N1
4	A	1002	CPS	C22-C23-C24-O1
4	C	1002	CPS	C22-C23-C24-N1
4	C	1002	CPS	C22-C23-C24-O1
4	C	1002	CPS	C22-C20-C9-C8
4	C	1002	CPS	C21-C20-C22-C23
4	C	1002	CPS	C21-C20-C9-C8
4	A	1002	CPS	C31-C32-S-O3S
3	C	1001	DEX	O4-C20-C21-O5
4	A	1002	CPS	C30-C31-C32-S
4	A	1002	CPS	C20-C22-C23-C24
4	C	1002	CPS	C22-C20-C9-C5
4	A	1002	CPS	C21-C20-C22-C23
3	E	1001	DEX	O4-C20-C21-O5
3	E	1001	DEX	C17-C20-C21-O5
4	C	1002	CPS	C26-C25-N1-C24
4	C	1002	CPS	C31-C30-N2-C27

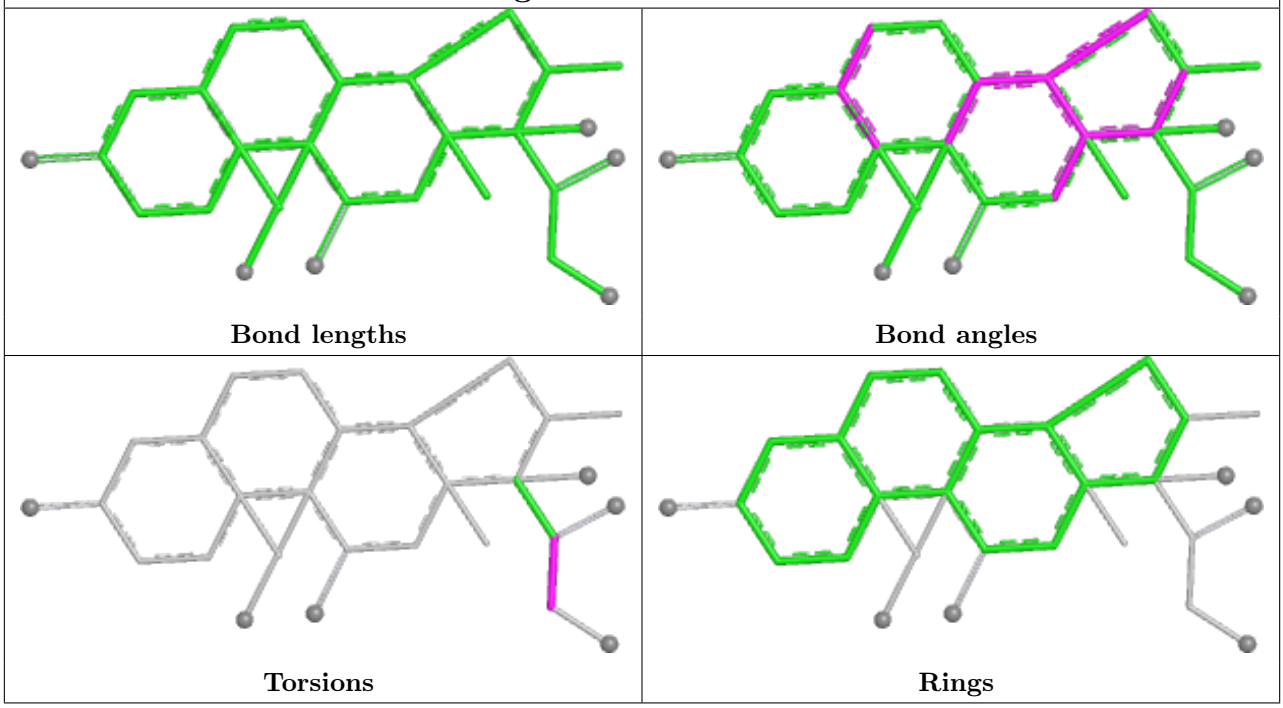
There are no ring outliers.

5 monomers are involved in 36 short contacts:

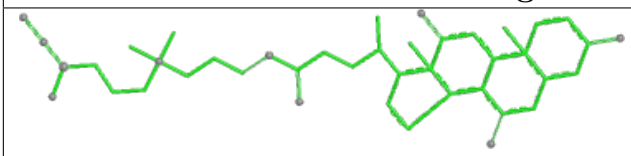
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	DEX	5	0
4	A	1002	CPS	21	0
4	C	1002	CPS	8	0
3	C	1001	DEX	1	0
3	E	1001	DEX	1	0

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 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.

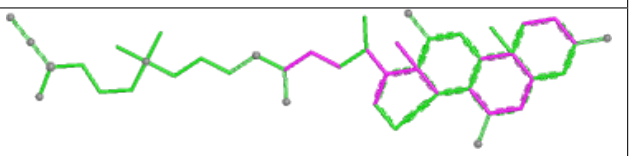
Ligand DEX A 1001



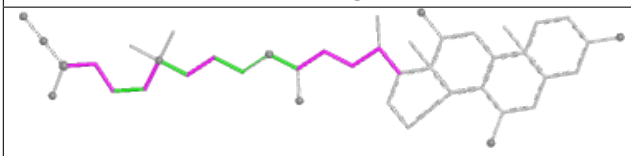
Ligand CPS A 1002



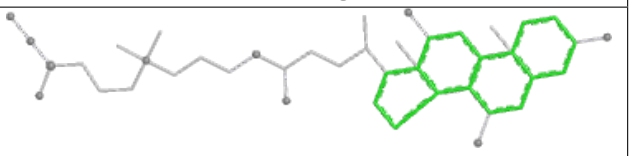
Bond lengths



Bond angles

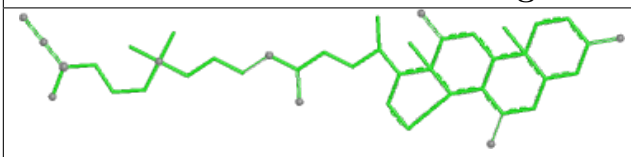


Torsions

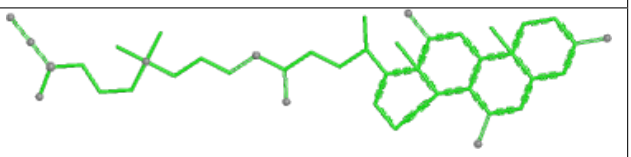


Rings

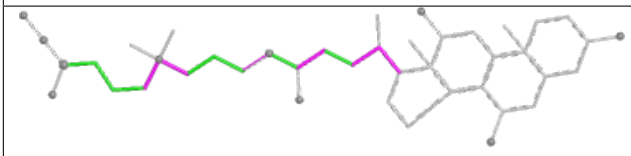
Ligand CPS C 1002



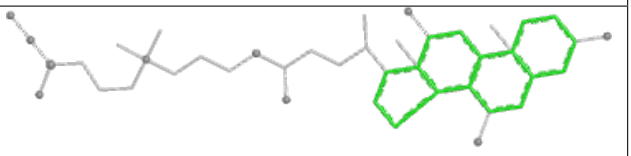
Bond lengths



Bond angles

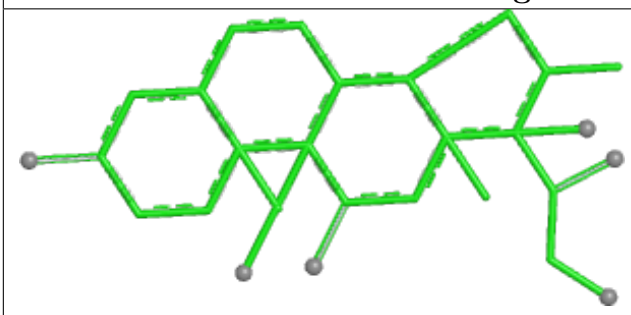


Torsions

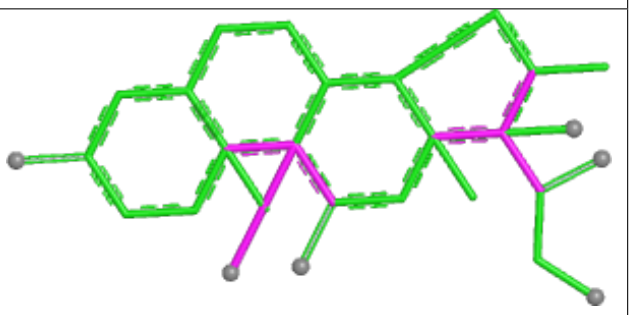


Rings

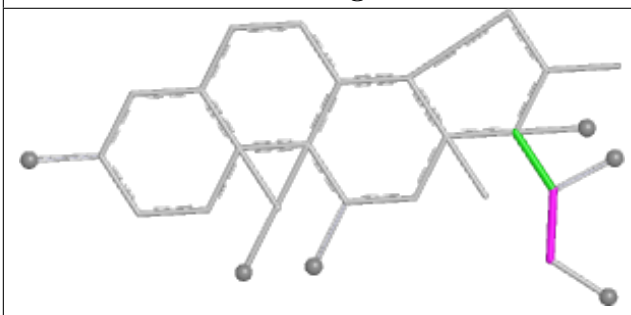
Ligand DEX C 1001



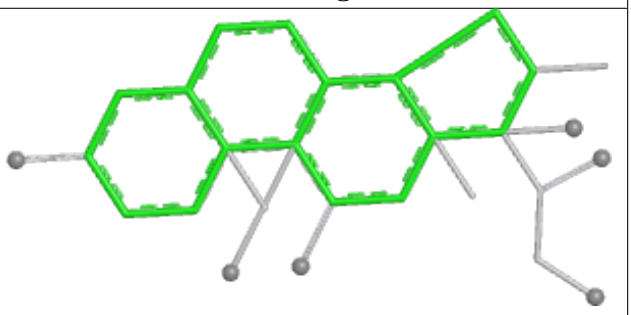
Bond lengths



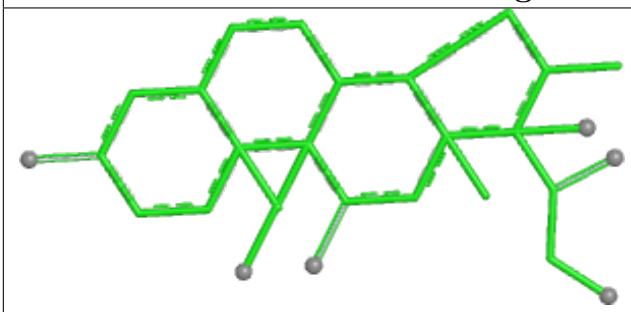
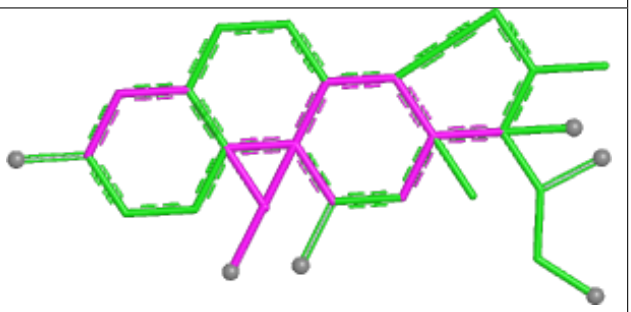
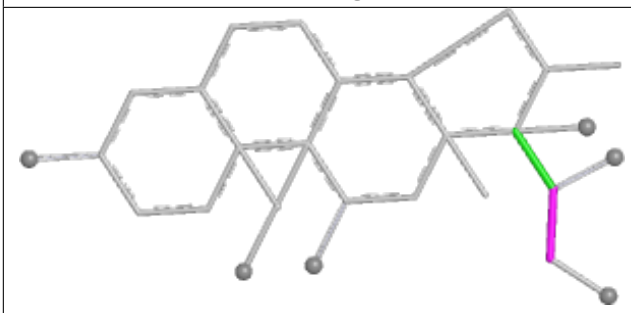
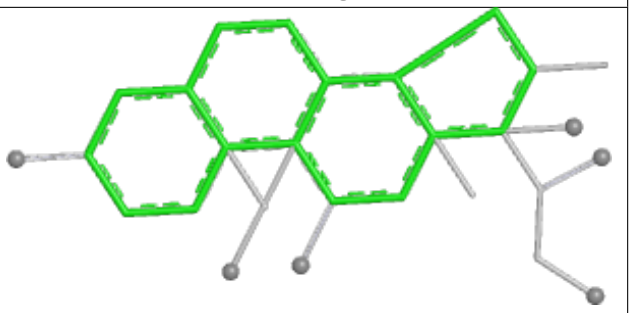
Bond angles



Torsions



Rings

Ligand DEX E 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	237/248 (95%)	0.54	11 (4%) 32 12	0, 63, 91, 147	0
1	C	237/248 (95%)	0.69	15 (6%) 20 6	0, 63, 100, 152	0
1	E	230/248 (92%)	0.88	35 (15%) 2 1	31, 71, 105, 139	0
2	B	10/11 (90%)	0.68	0 100 100	35, 58, 65, 73	0
2	D	9/11 (81%)	0.88	0 100 100	58, 63, 80, 83	0
2	F	9/11 (81%)	0.46	0 100 100	35, 47, 61, 63	0
All	All	732/777 (94%)	0.70	61 (8%) 11 3	0, 66, 101, 152	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	634	MET	5.3
1	E	718	LEU	4.7
1	E	555	THR	4.4
1	A	635	GLN	4.4
1	E	548	TYR	4.3
1	E	592	GLN	4.1
1	E	537	GLU	3.9
1	E	638	TYR	3.8
1	C	623	PHE	3.7
1	E	691	MET	3.6
1	E	660	TYR	3.4
1	A	559	LEU	3.3
1	E	653	PHE	3.2
1	E	680	LEU	3.2
1	E	543	VAL	3.1
1	C	627	LEU	2.9
1	E	655	ARG	2.9
1	E	666	MET	2.9
1	E	677	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	559	LEU	2.8
1	C	620	MET	2.8
1	E	772	LEU	2.7
1	C	618	GLY	2.7
1	A	610	TRP	2.7
1	C	745	LEU	2.7
1	A	623	PHE	2.6
1	E	650	SER	2.6
1	E	586	ASN	2.6
1	A	620	MET	2.5
1	C	761	LEU	2.5
1	C	720	LYS	2.5
1	E	582	PRO	2.5
1	E	536	LEU	2.5
1	A	634	MET	2.3
1	E	611	ARG	2.3
1	E	764	PHE	2.3
1	A	770	LYS	2.3
1	C	694	ILE	2.3
1	E	760	GLN	2.3
1	E	561	SER	2.3
1	C	588	HIS	2.3
1	E	647	LEU	2.2
1	C	638	TYR	2.2
1	E	654	VAL	2.2
1	E	656	LEU	2.2
1	E	596	LEU	2.2
1	A	735	PHE	2.2
1	C	725	MET	2.2
1	A	663	TYR	2.2
1	A	587	LEU	2.1
1	E	608	LEU	2.1
1	E	580	ALA	2.1
1	C	637	PRO	2.1
1	A	726	HIS	2.0
1	E	658	VAL	2.0
1	E	584	PHE	2.0
1	C	565	ARG	2.0
1	E	615	GLN	2.0
1	C	658	VAL	2.0
1	E	587	LEU	2.0
1	E	697	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

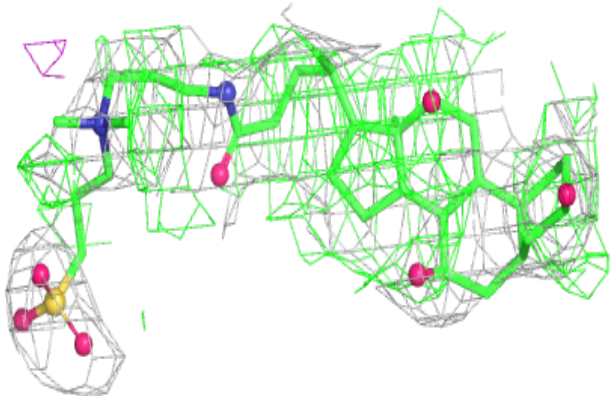
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

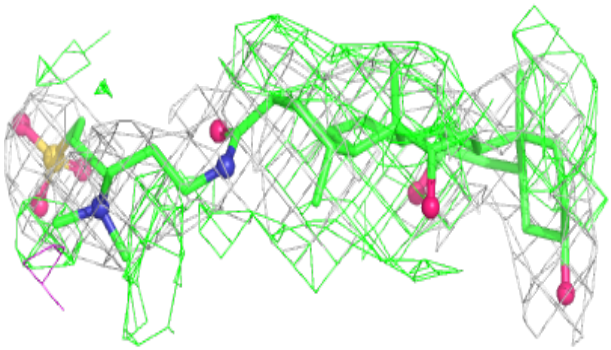
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CPS	A	1002	42/42	0.86	0.29	16,20,54,62	42
5	SO4	C	1004	5/5	0.88	0.15	98,99,114,117	0
4	CPS	C	1002	42/42	0.90	0.19	41,55,68,70	42
5	SO4	A	1003	5/5	0.92	0.15	113,113,119,122	5
3	DEX	A	1001	28/28	0.92	0.28	37,42,54,59	0
3	DEX	E	1001	28/28	0.94	0.29	50,64,73,89	0
5	SO4	C	1003	5/5	0.97	0.18	60,67,77,85	0
3	DEX	C	1001	28/28	0.97	0.36	50,59,68,77	0

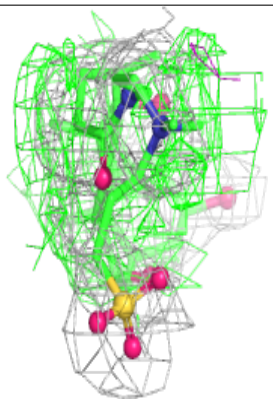
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPS A 1002:

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

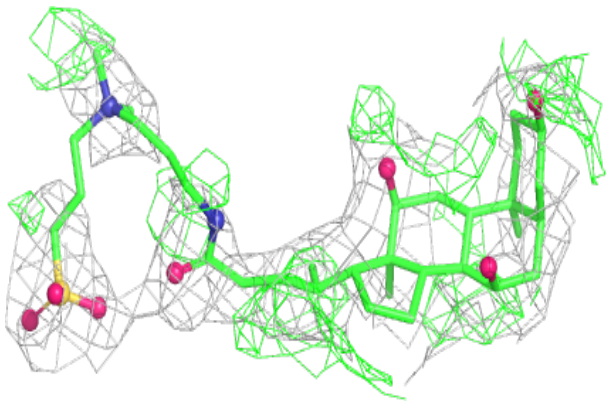


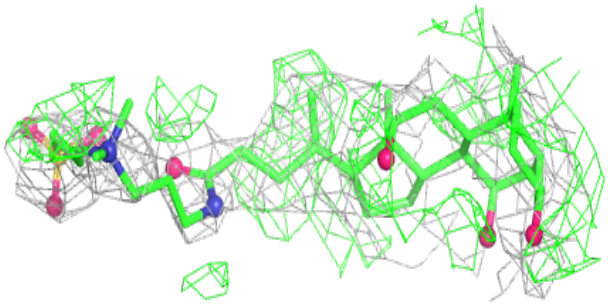


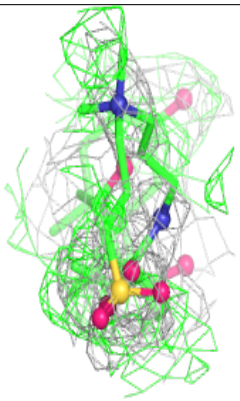


Electron density around CPS C 1002:

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

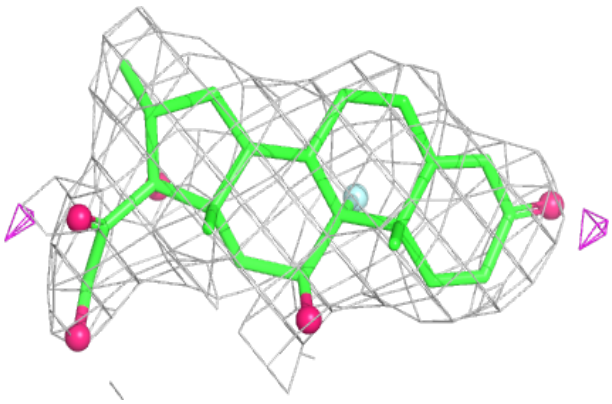


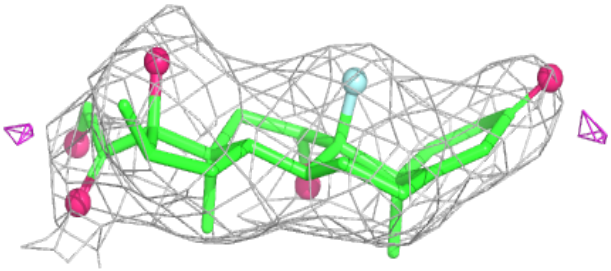


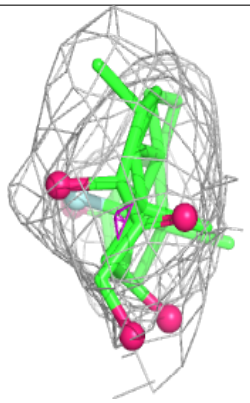


Electron density around DEX A 1001:

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

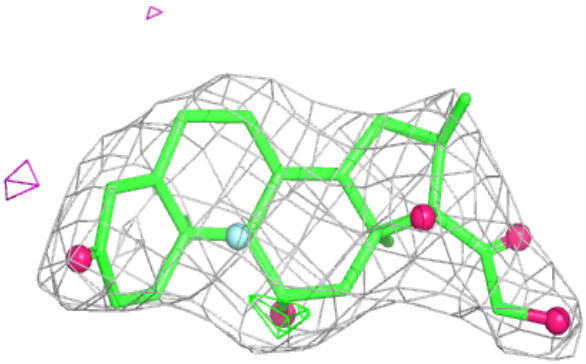


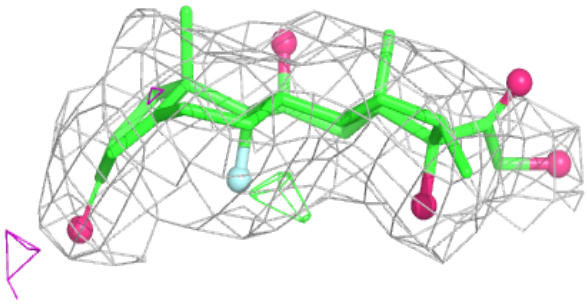


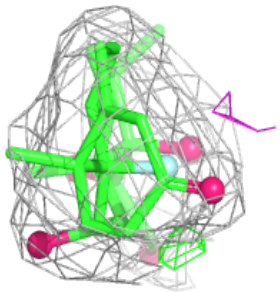


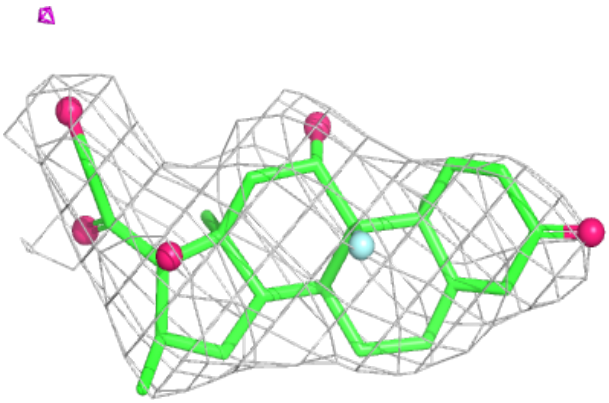
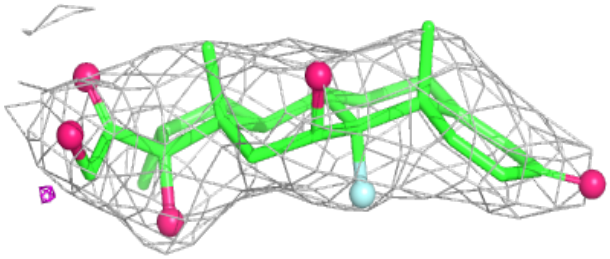
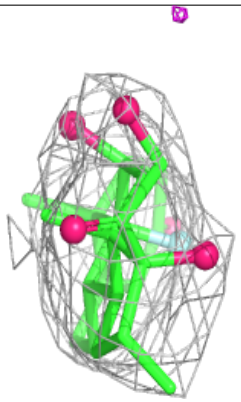
Electron density around DEX E 1001:

$2mF_o$-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.