Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 06:03 PM EST

PDB ID	:	1HDC
Title	:	MECHANISM OF INHIBITION OF 3ALPHA,20BETA-HYDROXYSTEROID DEHYDROGENASE BY A LICORICE-DERIVED STEROIDAL INHIBITOR
Authors	:	Ghosh, D.
Deposited on	:	1994-10-21
Resolution	:	2.20 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:

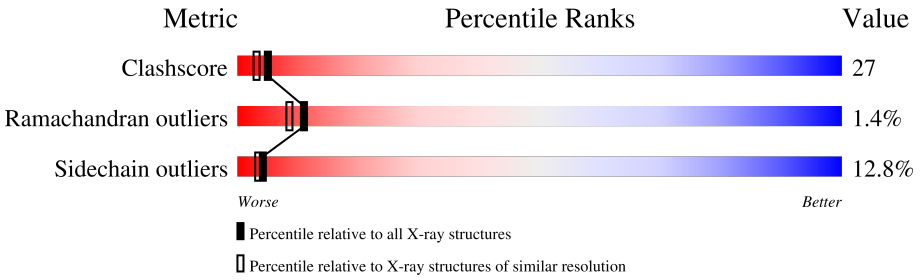
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	52% 41% 7%
1	B	254	54% 41% .
1	C	254	50% 43% 6%
1	D	254	50% 46% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7558 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.

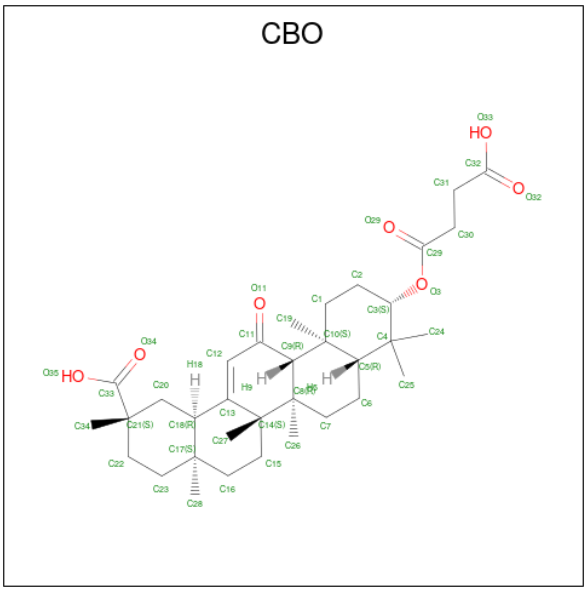
- Molecule 1 is a protein called 3-ALPHA, 20 BETA-HYDROXYSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1842	1144	323	367	8			
1	B	253	Total	C	N	O	S	0	0	0
			1842	1144	323	367	8			
1	C	253	Total	C	N	O	S	0	0	0
			1842	1144	323	367	8			
1	D	253	Total	C	N	O	S	0	0	0
			1842	1144	323	367	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	GLU	ASP	conflict	UNP P19992
B	109	GLU	ASP	conflict	UNP P19992
C	109	GLU	ASP	conflict	UNP P19992
D	109	GLU	ASP	conflict	UNP P19992

- Molecule 2 is CARBENOXOLONE (three-letter code: CBO) (formula: $C_{34}H_{50}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 41 34 7	0	0
2	B	1	Total C O 41 34 7	0	0
2	C	1	Total C O 41 34 7	0	0
2	D	1	Total C O 41 34 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	10	Total O 10 10	0	0
3	C	4	Total O 4 4	0	0
3	D	7	Total O 7 7	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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

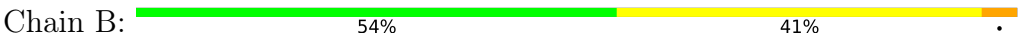
Note EDS was not executed.

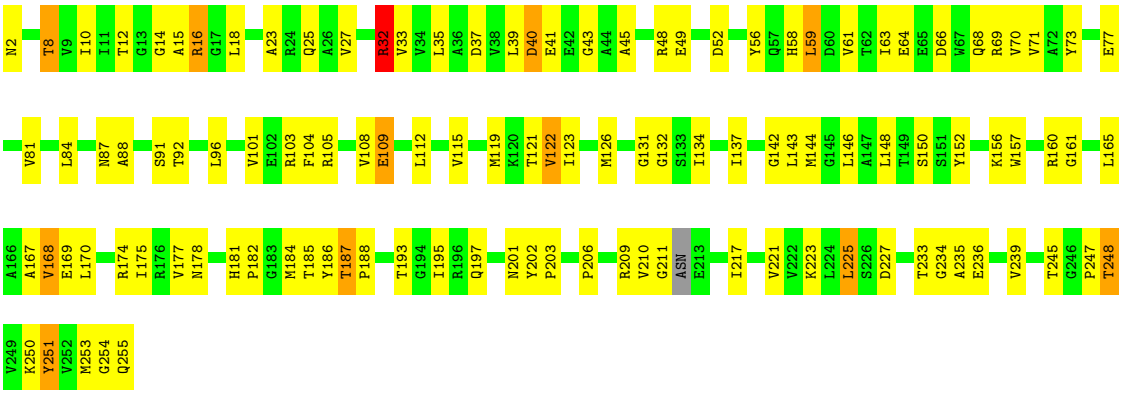
• Molecule 1: 3-ALPHA, 20 BETA-HYDROXYSTEROID DEHYDROGENASE

Chain A:

• Molecule 1: 3-ALPHA, 20 BETA-HYDROXYSTEROID DEHYDROGENASE

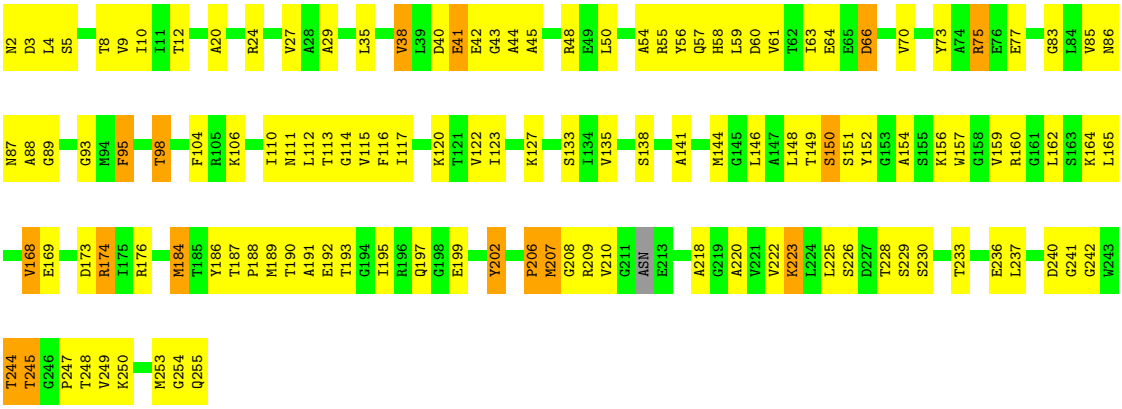
Chain B:





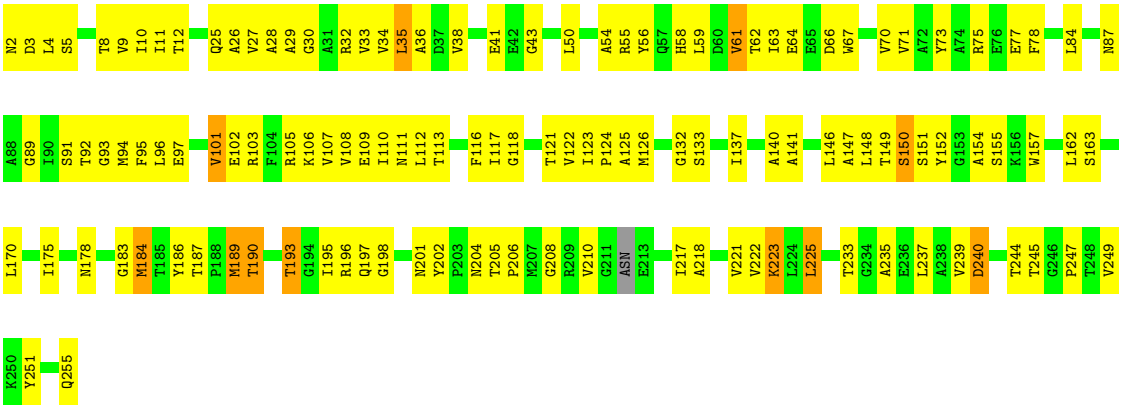
• Molecule 1: 3-ALPHA, 20 BETA-HYDROXYSTEROID DEHYDROGENASE

Chain C:



• Molecule 1: 3-ALPHA, 20 BETA-HYDROXYSTEROID DEHYDROGENASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.05Å 60.04Å 59.84Å 101.78° 104.41° 96.31°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7558	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.62	0/1867	0.85	1/2529 (0.0%)
1	B	0.60	0/1867	0.81	1/2529 (0.0%)
1	C	0.60	0/1867	0.85	1/2529 (0.0%)
1	D	0.60	0/1867	0.84	0/2529
All	All	0.60	0/7468	0.84	3/10116 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	225	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	14	GLY	N-CA-C	5.54	126.94	113.10
1	B	32	ARG	N-CA-C	-5.09	97.27	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	251	TYR	Sidechain

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	1842	0	1835	102	0
1	B	1842	0	1835	89	0
1	C	1842	0	1835	107	0
1	D	1842	0	1835	124	0
2	A	41	0	49	11	0
2	B	41	0	48	7	0
2	C	41	0	48	10	0
2	D	41	0	48	20	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	4	0	0	0	0
3	D	7	0	0	0	0
All	All	7558	0	7533	409	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 27.

All (409) 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:D:193:THR:HG21	2:D:301:CBO:H271	1.32	1.06
2:C:301:CBO:H192	2:C:301:CBO:H243	1.48	0.95
1:C:148:LEU:HD22	2:C:301:CBO:H282	1.51	0.93
1:C:27:VAL:HG21	1:C:50:LEU:HD13	1.51	0.92
1:C:250:LYS:HG3	1:C:255:GLN:HG3	1.58	0.86
1:A:223:LYS:HG3	1:D:223:LYS:HG3	1.56	0.85
1:B:91:SER:OG	2:B:301:CBO:H193	1.77	0.85
1:D:247:PRO:HB3	1:D:251:TYR:CD2	2.12	0.85
1:B:234:GLY:HA3	1:C:245:THR:HG21	1.62	0.82
1:C:174:ARG:HB2	1:C:174:ARG:NH1	1.93	0.82
1:D:71:VAL:HG21	1:D:121:THR:HG22	1.63	0.81
1:B:234:GLY:HA3	1:C:245:THR:CG2	2.11	0.81
1:D:59:LEU:HD12	1:D:70:VAL:HG21	1.64	0.80
1:A:69:ARG:HG3	1:A:69:ARG:HH11	1.48	0.77
1:B:223:LYS:HG3	1:C:223:LYS:HG3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASN:HD22	1:B:235:ALA:H	1.34	0.76
1:D:178:ASN:HD21	1:D:233:THR:HA	1.49	0.76
1:D:217:ILE:HD12	1:D:217:ILE:H	1.49	0.76
1:D:247:PRO:HB3	1:D:251:TYR:HD2	1.49	0.75
1:B:187:THR:HB	1:B:188:PRO:HD2	1.69	0.74
1:C:59:LEU:HD12	1:C:66:ASP:HB3	1.68	0.74
1:D:183:GLY:HA3	1:D:240:ASP:HB3	1.69	0.74
1:C:141:ALA:HB2	1:C:146:LEU:HD12	1.69	0.73
1:A:121:THR:O	1:A:124:PRO:HD2	1.88	0.73
1:B:160:ARG:HD3	1:B:181:HIS:HE1	1.54	0.73
1:C:2:ASN:HA	1:C:228:THR:OG1	1.89	0.72
1:B:12:THR:HG22	1:B:88:ALA:H	1.54	0.71
1:B:12:THR:O	1:B:87:ASN:HB3	1.90	0.71
1:D:12:THR:O	1:D:87:ASN:HB3	1.91	0.71
1:C:190:THR:O	1:C:195:ILE:HB	1.91	0.71
1:D:217:ILE:HD12	1:D:217:ILE:N	2.06	0.71
1:B:178:ASN:ND2	1:B:235:ALA:H	1.90	0.70
2:C:301:CBO:H192	2:C:301:CBO:C24	2.21	0.69
1:A:240:ASP:OD2	1:A:244:THR:HB	1.92	0.69
1:C:174:ARG:HB2	1:C:174:ARG:HH11	1.57	0.69
1:A:198:GLY:O	1:A:209:ARG:HB3	1.92	0.69
1:D:95:PHE:O	1:D:97:GLU:N	2.26	0.69
1:D:148:LEU:CB	2:D:301:CBO:H282	2.23	0.69
1:C:12:THR:HG22	1:C:88:ALA:HB2	1.75	0.68
1:B:143:LEU:HG	1:B:181:HIS:ND1	2.08	0.68
1:D:126:MET:SD	1:D:132:GLY:HA3	2.34	0.68
1:D:25:GLN:NE2	1:D:218:ALA:HB3	2.09	0.68
1:C:148:LEU:CD2	2:C:301:CBO:H282	2.22	0.68
1:D:108:VAL:HA	1:D:155:SER:OG	1.92	0.68
1:D:34:VAL:HG22	1:D:78:PHE:HE2	1.59	0.68
1:A:95:PHE:O	1:A:98:THR:HB	1.94	0.67
1:B:248:THR:HG22	1:B:251:TYR:H	1.60	0.66
1:D:84:LEU:HD22	1:D:122:VAL:HG11	1.78	0.66
2:D:301:CBO:H262	2:D:301:CBO:H162	1.76	0.66
1:B:184:MET:O	1:B:210:VAL:HG13	1.96	0.66
1:D:121:THR:O	1:D:124:PRO:HD2	1.95	0.66
1:A:119:MET:O	1:A:123:ILE:HG13	1.96	0.66
1:C:187:THR:HG22	1:C:190:THR:OG1	1.96	0.65
1:D:93:GLY:HA2	1:D:148:LEU:O	1.96	0.65
1:C:55:ARG:HE	1:C:77:GLU:HG2	1.61	0.65
1:C:250:LYS:HG3	1:C:255:GLN:CG	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:THR:O	1:C:87:ASN:HB3	1.97	0.64
1:C:93:GLY:HA2	1:C:148:LEU:O	1.97	0.64
1:D:148:LEU:HB2	2:D:301:CBO:H282	1.79	0.64
1:C:193:THR:HG23	2:C:301:CBO:H201	1.80	0.64
1:C:249:VAL:HG12	1:C:253:MET:SD	2.38	0.64
1:D:92:THR:O	1:D:149:THR:HA	1.98	0.64
1:A:50:LEU:HB2	1:A:54:ALA:CB	2.28	0.63
1:C:228:THR:O	1:C:228:THR:HG22	1.97	0.63
1:A:106:LYS:HE2	1:A:110:ILE:HD11	1.81	0.63
1:D:101:VAL:O	1:D:105:ARG:HG3	1.99	0.63
1:D:63:ILE:HG22	1:D:66:ASP:H	1.64	0.63
1:A:247:PRO:HB3	1:A:251:TYR:CD1	2.33	0.62
1:C:193:THR:HG21	2:C:301:CBO:H271	1.80	0.62
1:A:230:SER:O	1:A:231:TYR:HB2	1.99	0.62
1:D:178:ASN:HD22	1:D:235:ALA:H	1.48	0.62
1:B:64:GLU:HG2	1:B:68:GLN:OE1	2.00	0.61
1:D:59:LEU:HD21	1:D:61:VAL:HG23	1.82	0.61
1:A:242:GLY:O	1:A:245:THR:HG22	2.00	0.61
1:D:152:TYR:OH	2:D:301:CBO:H22	2.00	0.61
1:B:45:ALA:HA	1:B:48:ARG:NH1	2.15	0.61
1:B:169:GLU:HG2	1:D:147:ALA:HB1	1.83	0.60
1:A:16:ARG:HH21	1:A:188:PRO:HB2	1.66	0.60
1:A:36:ALA:HB1	1:A:59:LEU:HD23	1.82	0.60
1:B:63:ILE:HG22	1:B:66:ASP:H	1.67	0.60
1:B:217:ILE:N	1:B:217:ILE:HD12	2.17	0.59
1:A:162:LEU:HD13	1:C:154:ALA:HB2	1.85	0.59
1:B:160:ARG:HD3	1:B:181:HIS:CE1	2.35	0.59
1:C:24:ARG:HA	1:C:50:LEU:HD21	1.84	0.59
1:C:61:VAL:HG12	1:C:114:GLY:CA	2.33	0.59
1:C:38:VAL:HA	1:C:58:HIS:CE1	2.37	0.59
1:A:101:VAL:HG13	1:C:120:LYS:NZ	2.18	0.58
1:A:12:THR:HG22	1:A:88:ALA:CB	2.34	0.58
1:D:27:VAL:HG23	1:D:33:VAL:HG23	1.85	0.58
1:A:154:ALA:HB2	1:C:162:LEU:HD13	1.85	0.58
1:D:186:TYR:CD2	1:D:197:GLN:HB2	2.39	0.58
1:D:107:VAL:HG13	1:D:111:ASN:ND2	2.19	0.57
1:D:25:GLN:O	1:D:28:ALA:HB3	2.04	0.57
1:A:51:GLY:C	1:A:53:ALA:H	2.08	0.57
1:A:236:GLU:O	1:A:236:GLU:HG3	2.04	0.57
1:D:184:MET:HA	2:D:301:CBO:C25	2.35	0.57
1:C:35:LEU:N	1:C:35:LEU:HD23	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ALA:HA	1:B:48:ARG:CZ	2.34	0.57
1:D:148:LEU:HD12	2:D:301:CBO:H231	1.86	0.57
1:A:189:MET:HG3	1:A:190:THR:HG23	1.87	0.57
2:D:301:CBO:H283	2:D:301:CBO:H261	1.86	0.57
1:B:16:ARG:HD2	1:B:39:LEU:HD22	1.87	0.56
1:B:152:TYR:O	1:B:156:LYS:HG2	2.05	0.56
1:A:20:ALA:O	1:A:23:ALA:HB3	2.05	0.56
1:D:36:ALA:HB1	1:D:59:LEU:HD13	1.87	0.56
1:C:248:THR:HG22	1:C:250:LYS:H	1.69	0.56
1:D:55:ARG:HG3	1:D:78:PHE:CZ	2.41	0.56
1:C:189:MET:HA	1:C:192:GLU:HB2	1.88	0.56
1:D:34:VAL:CG2	1:D:78:PHE:HE2	2.17	0.55
1:D:71:VAL:HG21	1:D:121:THR:CG2	2.34	0.55
1:B:134:ILE:HD12	1:B:177:VAL:HG22	1.89	0.55
1:C:44:ALA:O	1:C:48:ARG:HG3	2.06	0.55
1:B:81:VAL:O	1:B:126:MET:HG2	2.06	0.55
1:C:220:ALA:HB1	1:C:237:LEU:HD23	1.87	0.55
2:C:301:CBO:H271	2:C:301:CBO:H202	1.89	0.55
1:B:119:MET:HE3	1:B:134:ILE:HD13	1.89	0.55
1:C:160:ARG:HD2	1:C:236:GLU:OE1	2.06	0.55
1:B:167:ALA:HB1	1:B:233:THR:HG22	1.89	0.55
1:A:189:MET:HE2	1:A:190:THR:HG22	1.88	0.54
1:A:2:ASN:HB3	1:D:3:ASP:H	1.72	0.54
1:B:73:TYR:O	1:B:77:GLU:HB2	2.07	0.54
1:B:187:THR:HB	1:B:188:PRO:CD	2.36	0.54
1:D:93:GLY:O	1:D:94:MET:HB3	2.07	0.54
1:B:148:LEU:HD13	2:B:301:CBO:H282	1.90	0.54
1:C:218:ALA:O	1:C:222:VAL:HG23	2.08	0.54
1:B:8:THR:HB	1:B:32:ARG:HB2	1.89	0.54
1:C:141:ALA:CB	1:C:146:LEU:HD12	2.37	0.54
1:A:173:ASP:O	1:A:175:ILE:HD12	2.08	0.54
1:A:250:LYS:HG2	1:A:255:GLN:HG3	1.89	0.54
1:D:198:GLY:O	1:D:201:ASN:HB2	2.08	0.54
1:C:148:LEU:HD11	1:D:249:VAL:HG13	1.90	0.54
1:B:245:THR:HG23	1:C:164:LYS:HB3	1.89	0.53
1:C:199:GLU:OE2	1:C:209:ARG:HD3	2.07	0.53
1:C:24:ARG:HA	1:C:50:LEU:CD2	2.38	0.53
1:A:91:SER:HB2	2:A:301:CBO:H193	1.90	0.53
1:B:178:ASN:HD22	1:B:235:ALA:N	2.03	0.53
1:B:247:PRO:HB3	1:B:251:TYR:CD1	2.44	0.53
1:C:27:VAL:CG2	1:C:50:LEU:HD13	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:O	1:C:115:VAL:HG22	2.08	0.53
2:B:301:CBO:H192	2:B:301:CBO:H243	1.91	0.53
1:C:186:TYR:CE1	1:C:197:GLN:HB3	2.43	0.53
1:D:148:LEU:HB3	2:D:301:CBO:C28	2.39	0.53
1:C:50:LEU:HB2	1:C:54:ALA:HB2	1.90	0.53
1:D:196:ARG:HB3	1:D:201:ASN:HB3	1.90	0.53
1:D:27:VAL:HG23	1:D:33:VAL:CG2	2.39	0.53
1:D:148:LEU:HB3	2:D:301:CBO:H282	1.90	0.53
1:D:43:GLY:HA3	1:D:56:TYR:CE1	2.44	0.53
1:A:2:ASN:HB3	1:D:2:ASN:OD1	2.09	0.52
1:A:247:PRO:HD3	1:B:144:MET:SD	2.49	0.52
1:B:104:PHE:O	1:B:108:VAL:HG23	2.10	0.52
1:D:33:VAL:HG12	1:D:35:LEU:HD23	1.90	0.52
1:B:168:VAL:HG21	1:C:247:PRO:O	2.09	0.52
1:C:165:LEU:O	1:C:169:GLU:HG3	2.08	0.52
1:D:91:SER:HA	1:D:152:TYR:CD1	2.45	0.52
1:C:83:GLY:HA2	1:C:133:SER:O	2.10	0.52
1:A:134:ILE:HB	1:A:177:VAL:HG13	1.90	0.52
1:B:161:GLY:HA3	1:D:157:TRP:CG	2.44	0.52
1:D:202:TYR:O	1:D:205:THR:HG22	2.10	0.52
1:A:134:ILE:HD12	1:A:177:VAL:HG22	1.90	0.52
1:D:217:ILE:H	1:D:217:ILE:CD1	2.19	0.52
1:A:18:LEU:HD21	1:A:217:ILE:HB	1.90	0.52
1:D:183:GLY:CA	1:D:240:ASP:HB3	2.37	0.52
1:D:187:THR:HG22	1:D:190:THR:OG1	2.10	0.52
1:D:184:MET:HA	2:D:301:CBO:H251	1.90	0.51
1:D:196:ARG:HG2	1:D:196:ARG:HH11	1.76	0.51
1:D:43:GLY:HA3	1:D:56:TYR:CD1	2.45	0.51
1:A:138:SER:HA	1:A:156:LYS:HD2	1.92	0.51
1:D:26:ALA:O	1:D:29:ALA:HB3	2.10	0.51
1:D:113:THR:HG22	1:D:117:ILE:HG13	1.92	0.51
1:A:50:LEU:HB2	1:A:54:ALA:HB2	1.92	0.51
1:A:137:ILE:HD13	1:A:180:VAL:HB	1.92	0.51
1:B:84:LEU:HD22	1:B:122:VAL:HG11	1.92	0.51
1:A:75:ARG:HG3	1:A:80:SER:HA	1.93	0.51
1:B:187:THR:CB	1:B:188:PRO:HD2	2.40	0.51
1:D:54:ALA:O	1:D:55:ARG:HG2	2.10	0.51
1:D:187:THR:HG23	1:D:189:MET:H	1.74	0.51
1:A:195:ILE:HG23	1:A:210:VAL:HG11	1.93	0.51
1:C:55:ARG:HB3	1:C:73:TYR:OH	2.11	0.51
1:D:205:THR:HG23	1:D:208:GLY:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:TYR:O	1:C:156:LYS:HG2	2.11	0.51
1:D:73:TYR:CZ	1:D:77:GLU:HG3	2.46	0.51
1:D:202:TYR:HB2	1:D:210:VAL:HG23	1.93	0.50
1:D:103:ARG:HG3	1:D:106:LYS:NZ	2.26	0.50
1:C:41:GLU:CD	1:C:41:GLU:H	2.15	0.50
1:D:73:TYR:O	1:D:77:GLU:HG2	2.11	0.50
1:C:104:PHE:CD2	1:C:151:SER:HB3	2.47	0.50
1:B:91:SER:HG	2:B:301:CBO:H193	1.75	0.50
1:D:36:ALA:CB	1:D:59:LEU:HD13	2.42	0.50
1:D:205:THR:HG23	1:D:208:GLY:N	2.27	0.50
1:D:218:ALA:O	1:D:222:VAL:HG23	2.11	0.50
1:D:11:ILE:HD12	1:D:33:VAL:CG1	2.42	0.50
1:D:92:THR:HA	1:D:103:ARG:NH2	2.26	0.50
1:C:4:LEU:HA	1:C:29:ALA:HB1	1.94	0.50
1:C:5:SER:N	1:C:29:ALA:O	2.44	0.50
1:A:51:GLY:O	1:A:53:ALA:N	2.45	0.50
1:D:193:THR:HB	1:D:195:ILE:HD11	1.93	0.50
1:B:58:HIS:O	1:B:69:ARG:NH2	2.44	0.49
1:C:57:GLN:HG3	1:C:70:VAL:HG13	1.94	0.49
1:C:190:THR:O	1:C:193:THR:HB	2.11	0.49
1:B:59:LEU:HG	1:B:70:VAL:HG21	1.94	0.49
1:B:112:LEU:O	1:B:115:VAL:HG22	2.13	0.49
1:B:168:VAL:HG22	1:D:147:ALA:HB2	1.94	0.49
1:A:101:VAL:HG13	1:C:120:LYS:HZ1	1.78	0.49
1:B:160:ARG:NH1	1:B:236:GLU:OE2	2.46	0.49
1:C:254:GLY:HA2	1:D:204:ASN:ND2	2.28	0.49
1:B:142:GLY:HA2	1:B:157:TRP:CD1	2.47	0.49
2:B:301:CBO:H263	2:B:301:CBO:H191	1.95	0.49
1:C:164:LYS:O	1:C:168:VAL:HG12	2.12	0.49
1:A:55:ARG:HG2	1:A:78:PHE:HZ	1.77	0.49
1:B:2:ASN:HA	1:C:3:ASP:HB2	1.95	0.49
1:B:193:THR:HG23	2:B:301:CBO:H343	1.95	0.49
1:C:9:VAL:HG23	1:C:83:GLY:C	2.33	0.49
1:A:15:ALA:HB3	1:A:37:ASP:OD2	2.13	0.49
1:A:45:ALA:O	1:A:48:ARG:HB3	2.12	0.49
1:A:170:LEU:HB3	1:A:175:ILE:HB	1.93	0.49
1:B:45:ALA:O	1:B:48:ARG:HB3	2.12	0.49
1:D:178:ASN:HD21	1:D:233:THR:CA	2.22	0.49
2:A:301:CBO:H263	2:A:301:CBO:H191	1.94	0.48
1:C:89:GLY:CA	1:C:111:ASN:OD1	2.61	0.48
1:C:89:GLY:HA3	1:C:111:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:MET:HG2	1:C:202:TYR:CE2	2.48	0.48
1:A:148:LEU:HD13	2:A:301:CBO:H282	1.96	0.48
1:C:188:PRO:O	1:C:191:ALA:HB3	2.13	0.48
1:D:152:TYR:CE2	2:D:301:CBO:H192	2.48	0.48
1:A:55:ARG:CG	1:A:78:PHE:HZ	2.27	0.48
1:D:38:VAL:HA	1:D:58:HIS:CE1	2.49	0.48
1:D:193:THR:HG22	2:D:301:CBO:H343	1.96	0.48
1:A:73:TYR:CD1	1:A:73:TYR:C	2.87	0.48
1:D:55:ARG:CG	1:D:78:PHE:HZ	2.26	0.48
1:D:147:ALA:O	1:D:148:LEU:HB2	2.14	0.48
1:D:149:THR:O	1:D:152:TYR:HB3	2.14	0.48
1:B:132:GLY:O	1:B:175:ILE:HA	2.14	0.48
2:D:301:CBO:H162	2:D:301:CBO:C26	2.44	0.48
1:B:81:VAL:HG11	1:B:122:VAL:CG2	2.43	0.47
1:D:184:MET:O	1:D:210:VAL:HG13	2.14	0.47
1:A:178:ASN:HD22	1:A:235:ALA:H	1.62	0.47
1:D:217:ILE:N	1:D:217:ILE:CD1	2.77	0.47
1:A:184:MET:CE	2:A:301:CBO:H3	2.44	0.47
1:D:116:PHE:HB2	1:D:162:LEU:HD21	1.97	0.47
1:A:187:THR:HG22	1:A:190:THR:OG1	2.13	0.47
1:A:55:ARG:CG	1:A:78:PHE:CZ	2.98	0.47
1:A:55:ARG:HG3	1:A:78:PHE:CE2	2.50	0.47
1:C:174:ARG:HB2	1:C:174:ARG:CZ	2.45	0.47
1:C:193:THR:HG21	2:C:301:CBO:C27	2.43	0.47
1:A:242:GLY:HA2	1:A:245:THR:HG22	1.96	0.47
1:C:63:ILE:HG22	1:C:66:ASP:H	1.79	0.47
1:C:75:ARG:HB2	1:C:75:ARG:HH11	1.80	0.47
1:B:221:VAL:HG12	1:B:225:LEU:HD22	1.97	0.47
1:D:202:TYR:HB2	1:D:210:VAL:CG2	2.45	0.46
1:A:242:GLY:CA	1:A:245:THR:HG22	2.45	0.46
1:B:186:TYR:HE1	1:B:195:ILE:O	1.98	0.46
1:C:60:ASP:OD2	1:C:63:ILE:HG12	2.14	0.46
1:D:193:THR:CG2	2:D:301:CBO:H202	2.44	0.46
1:A:2:ASN:OD1	1:A:2:ASN:N	2.49	0.46
1:A:148:LEU:N	1:A:148:LEU:HD23	2.30	0.46
1:B:178:ASN:ND2	1:B:235:ALA:HB3	2.30	0.46
1:B:254:GLY:C	1:B:255:GLN:NE2	2.69	0.46
1:C:89:GLY:HA2	1:C:110:ILE:HG22	1.97	0.46
1:D:75:ARG:NH2	1:D:125:ALA:HA	2.31	0.46
1:C:207:MET:HB2	1:C:241:GLY:O	2.15	0.46
1:D:67:TRP:O	1:D:71:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:OE1	1:A:255:GLN:N	2.49	0.46
1:B:8:THR:HB	1:B:32:ARG:CG	2.45	0.46
1:B:92:THR:HG23	1:B:103:ARG:HH21	1.81	0.46
1:B:105:ARG:O	1:B:109:GLU:HB2	2.15	0.46
1:B:112:LEU:HD21	1:D:154:ALA:HB1	1.97	0.46
1:B:202:TYR:HB2	1:B:210:VAL:HG23	1.97	0.46
1:C:63:ILE:HB	1:C:66:ASP:HB2	1.98	0.46
1:C:186:TYR:OH	1:C:197:GLN:NE2	2.48	0.46
1:D:50:LEU:HD12	1:D:54:ALA:HB2	1.98	0.46
1:D:193:THR:HG21	2:D:301:CBO:C27	2.23	0.46
1:C:55:ARG:HH21	1:C:77:GLU:CD	2.20	0.45
1:D:67:TRP:CE2	1:D:118:GLY:HA2	2.51	0.45
1:C:202:TYR:O	1:C:208:GLY:HA2	2.17	0.45
2:D:301:CBO:H271	2:D:301:CBO:H202	1.98	0.45
1:B:14:GLY:O	1:B:35:LEU:HD22	2.16	0.45
1:C:115:VAL:HG21	1:C:159:VAL:HG22	1.97	0.45
2:C:301:CBO:H263	2:C:301:CBO:H191	1.98	0.45
2:D:301:CBO:H263	2:D:301:CBO:H191	1.98	0.45
1:B:40:ASP:HA	1:B:56:TYR:CZ	2.52	0.45
1:D:87:ASN:ND2	1:D:87:ASN:O	2.49	0.45
1:A:63:ILE:O	1:A:66:ASP:HB2	2.16	0.45
1:B:43:GLY:HA3	1:B:56:TYR:CE1	2.52	0.45
1:C:195:ILE:HG23	1:C:210:VAL:HG11	1.99	0.45
1:A:69:ARG:HH11	1:A:69:ARG:CG	2.23	0.45
1:A:92:THR:OG1	1:A:103:ARG:NH2	2.49	0.45
2:A:301:CBO:H162	1:B:253:MET:HG2	1.98	0.45
1:B:123:ILE:HD11	1:B:170:LEU:HD11	1.97	0.45
1:D:197:GLN:HG2	1:D:198:GLY:N	2.32	0.45
1:A:123:ILE:HD13	1:A:170:LEU:HD21	1.99	0.45
1:C:106:LYS:HA	1:C:106:LYS:HD2	1.76	0.45
1:A:62:THR:HG21	1:A:109:GLU:HG3	1.99	0.44
1:B:168:VAL:HA	1:C:206:PRO:HB3	1.99	0.44
1:B:254:GLY:O	1:B:255:GLN:HB2	2.17	0.44
1:A:106:LYS:O	1:A:110:ILE:HG13	2.17	0.44
1:A:184:MET:HE3	2:A:301:CBO:H3	1.99	0.44
1:A:187:THR:HG23	1:A:190:THR:H	1.82	0.44
1:A:69:ARG:HG3	1:A:69:ARG:NH1	2.25	0.44
2:A:301:CBO:H271	2:A:301:CBO:H202	1.98	0.44
1:B:87:ASN:HD22	1:B:137:ILE:HG13	1.82	0.44
1:C:95:PHE:O	1:C:98:THR:HB	2.17	0.44
1:C:176:ARG:HG2	1:C:233:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLY:HA2	1:A:148:LEU:O	2.16	0.44
1:A:204:ASN:HD21	1:B:255:GLN:HE22	1.66	0.44
1:A:205:THR:HG21	1:A:209:ARG:O	2.17	0.44
1:B:156:LYS:HD3	1:B:156:LYS:HA	1.78	0.44
1:A:237:LEU:HD13	1:D:237:LEU:HD13	2.00	0.44
1:B:23:ALA:HB2	1:B:35:LEU:HD21	2.00	0.44
1:D:107:VAL:HB	1:D:151:SER:HB2	1.99	0.44
1:A:164:LYS:O	1:A:168:VAL:HG12	2.18	0.44
1:C:193:THR:HB	1:C:195:ILE:HD13	2.00	0.44
1:D:193:THR:HG22	2:D:301:CBO:C34	2.48	0.43
1:B:71:VAL:HG21	1:B:121:THR:HG22	2.00	0.43
1:A:8:THR:HG21	1:A:80:SER:O	2.19	0.43
1:A:86:ASN:ND2	1:A:115:VAL:HB	2.32	0.43
1:A:136:ASN:HB3	1:A:159:VAL:CG1	2.49	0.43
1:A:229:SER:O	1:A:231:TYR:N	2.50	0.43
1:B:161:GLY:HA3	1:D:157:TRP:CD1	2.53	0.43
1:B:165:LEU:O	1:B:169:GLU:HG3	2.18	0.43
1:B:193:THR:HG23	2:B:301:CBO:H202	2.00	0.43
1:C:113:THR:O	1:C:116:PHE:HB3	2.18	0.43
1:D:141:ALA:HB2	1:D:146:LEU:HD12	2.01	0.43
1:A:12:THR:HG22	1:A:88:ALA:HB2	1.99	0.43
1:B:15:ALA:HB3	1:B:37:ASP:OD2	2.19	0.43
1:C:38:VAL:HG23	1:C:59:LEU:O	2.18	0.43
1:C:138:SER:HA	1:C:156:LYS:HD2	2.00	0.43
1:A:173:ASP:HA	1:A:174:ARG:HH21	1.83	0.43
1:D:92:THR:HG23	1:D:94:MET:HE3	2.01	0.43
1:A:2:ASN:CB	1:D:2:ASN:HA	2.48	0.43
1:B:131:GLY:HA3	1:B:174:ARG:HB2	2.01	0.43
1:D:140:ALA:HB2	1:D:183:GLY:HA2	2.01	0.43
1:A:162:LEU:HD12	1:A:165:LEU:HD21	2.00	0.43
1:C:184:MET:HG2	1:C:202:TYR:HE2	1.83	0.43
1:B:248:THR:CG2	1:B:250:LYS:HB3	2.48	0.43
1:C:43:GLY:HA3	1:C:56:TYR:CD1	2.54	0.43
1:C:64:GLU:HA	1:C:117:ILE:HG21	2.01	0.43
1:A:93:GLY:CA	2:A:301:CBO:H261	2.50	0.42
1:D:11:ILE:HD12	1:D:33:VAL:HG11	2.00	0.42
1:D:205:THR:HG23	1:D:205:THR:O	2.18	0.42
1:A:9:VAL:HG23	1:A:9:VAL:O	2.20	0.42
1:C:174:ARG:HH11	1:C:174:ARG:CB	2.27	0.42
1:C:123:ILE:CG2	1:C:127:LYS:HE3	2.50	0.42
1:D:123:ILE:HD11	1:D:170:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD12	1:A:4:LEU:HA	1.81	0.42
1:A:237:LEU:HG	1:A:238:ALA:N	2.34	0.42
1:C:156:LYS:HA	1:C:156:LYS:HD3	1.74	0.42
1:D:62:THR:HG21	1:D:109:GLU:HG3	2.01	0.42
1:A:59:LEU:HD12	1:A:60:ASP:N	2.34	0.42
1:A:37:ASP:OD1	1:A:38:VAL:N	2.51	0.42
1:A:68:GLN:HE21	1:A:68:GLN:HB2	1.67	0.42
1:C:61:VAL:HG12	1:C:114:GLY:HA2	2.00	0.42
1:C:240:ASP:OD2	1:C:244:THR:HB	2.19	0.42
1:C:95:PHE:CD1	1:C:95:PHE:N	2.86	0.42
1:D:5:SER:O	1:D:30:GLY:C	2.57	0.42
1:D:225:LEU:HD12	1:D:225:LEU:HA	1.85	0.42
1:A:2:ASN:HB2	1:D:2:ASN:HA	2.01	0.42
1:A:3:ASP:HB3	1:A:226:SER:OG	2.19	0.42
1:B:217:ILE:N	1:B:217:ILE:CD1	2.83	0.42
1:A:164:LYS:HD2	1:C:157:TRP:CZ2	2.54	0.42
1:A:51:GLY:C	1:A:53:ALA:N	2.73	0.41
1:B:23:ALA:CB	1:B:35:LEU:HD21	2.50	0.41
1:C:20:ALA:O	1:C:24:ARG:HG3	2.20	0.41
1:C:42:GLU:O	1:C:45:ALA:HB3	2.20	0.41
1:C:149:THR:O	1:C:150:SER:C	2.58	0.41
1:C:223:LYS:NZ	1:C:229:SER:HB3	2.34	0.41
1:D:2:ASN:OD1	1:D:3:ASP:N	2.53	0.41
1:D:170:LEU:HB3	1:D:175:ILE:HB	2.01	0.41
1:A:66:ASP:O	1:A:70:VAL:HG23	2.21	0.41
1:A:148:LEU:CD1	2:A:301:CBO:H282	2.50	0.41
1:D:36:ALA:HB1	1:D:59:LEU:HB3	2.02	0.41
1:D:217:ILE:HA	1:D:239:VAL:HG11	2.02	0.41
1:A:189:MET:HE1	2:A:301:CBO:H11	2.02	0.41
1:A:250:LYS:CG	1:A:255:GLN:HG3	2.49	0.41
1:B:182:PRO:HA	1:B:239:VAL:O	2.20	0.41
2:C:301:CBO:H271	2:C:301:CBO:C20	2.50	0.41
1:D:55:ARG:CG	1:D:78:PHE:CZ	3.03	0.41
1:D:64:GLU:HA	1:D:67:TRP:HB2	2.00	0.41
1:D:89:GLY:HA2	1:D:110:ILE:HG22	2.01	0.41
1:D:108:VAL:O	1:D:112:LEU:HB3	2.21	0.41
2:D:301:CBO:C2	2:D:301:CBO:H302	2.50	0.41
1:A:93:GLY:HA2	2:A:301:CBO:H261	2.02	0.41
1:C:85:VAL:HA	1:C:135:VAL:O	2.19	0.41
1:C:220:ALA:HB1	1:C:237:LEU:CD2	2.51	0.41
1:A:36:ALA:CB	1:A:59:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LEU:HD12	1:B:39:LEU:N	2.35	0.41
1:D:73:TYR:CE1	1:D:77:GLU:HG3	2.56	0.41
1:D:106:LYS:HE2	1:D:106:LYS:HB3	1.85	0.41
1:A:12:THR:HG22	1:A:88:ALA:HB3	2.01	0.41
1:A:116:PHE:CZ	1:A:120:LYS:HD2	2.56	0.41
1:D:137:ILE:HD11	1:D:221:VAL:HG22	2.03	0.41
1:A:16:ARG:HH21	1:A:188:PRO:CB	2.34	0.41
1:B:92:THR:HG23	1:B:103:ARG:NH2	2.36	0.41
1:B:185:THR:HG23	1:B:211:GLY:O	2.20	0.41
1:C:254:GLY:O	1:C:255:GLN:HB2	2.20	0.41
1:A:7:LYS:HA	1:A:32:ARG:HH21	1.86	0.41
1:B:12:THR:HG22	1:B:88:ALA:N	2.30	0.41
1:D:108:VAL:O	1:D:112:LEU:N	2.53	0.41
1:A:55:ARG:HG3	1:A:78:PHE:CZ	2.56	0.40
1:C:86:ASN:HB3	1:C:115:VAL:HG12	2.02	0.40
1:D:11:ILE:HD12	1:D:33:VAL:HG13	2.03	0.40
1:B:201:ASN:C	1:B:203:PRO:HD3	2.41	0.40
1:A:97:GLU:HA	1:C:120:LYS:HG3	2.03	0.40
1:B:66:ASP:O	1:B:70:VAL:HG23	2.21	0.40
1:B:197:GLN:O	1:B:201:ASN:ND2	2.54	0.40
1:C:242:GLY:HA2	1:C:245:THR:HG23	2.02	0.40
1:D:149:THR:O	1:D:150:SER:C	2.60	0.40
1:A:71:VAL:HG21	1:A:121:THR:HG22	2.04	0.40
1:B:27:VAL:HG23	1:B:33:VAL:HG21	2.03	0.40
1:C:141:ALA:CA	1:C:146:LEU:HD12	2.50	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	251/254 (99%)	225 (90%)	19 (8%)	7 (3%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	251/254 (99%)	230 (92%)	19 (8%)	2 (1%)	19 19
1	C	251/254 (99%)	233 (93%)	16 (6%)	2 (1%)	19 19
1	D	251/254 (99%)	221 (88%)	27 (11%)	3 (1%)	13 10
All	All	1004/1016 (99%)	909 (90%)	81 (8%)	14 (1%)	11 8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	TYR
1	C	150	SER
1	C	184	MET
1	D	96	LEU
1	D	150	SER
1	A	52	ASP
1	A	184	MET
1	B	150	SER
1	A	18	LEU
1	A	150	SER
1	A	230	SER
1	D	184	MET
1	B	40	ASP
1	A	61	VAL

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	187/188 (100%)	158 (84%)	29 (16%)	2 2
1	B	187/188 (100%)	164 (88%)	23 (12%)	4 4
1	C	187/188 (100%)	165 (88%)	22 (12%)	5 4
1	D	187/188 (100%)	165 (88%)	22 (12%)	5 4
All	All	748/752 (100%)	652 (87%)	96 (13%)	4 3

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	7	LYS
1	A	8	THR
1	A	10	ILE
1	A	18	LEU
1	A	41	GLU
1	A	61	VAL
1	A	69	ARG
1	A	73	TYR
1	A	80	SER
1	A	96	LEU
1	A	102	GLU
1	A	103	ARG
1	A	122	VAL
1	A	128	ASP
1	A	146	LEU
1	A	155	SER
1	A	172	THR
1	A	174	ARG
1	A	189	MET
1	A	192	GLU
1	A	206	PRO
1	A	209	ARG
1	A	223	LYS
1	A	227	ASP
1	A	229	SER
1	A	233	THR
1	A	244	THR
1	A	248	THR
1	B	8	THR
1	B	10	ILE
1	B	16	ARG
1	B	18	LEU
1	B	25	GLN
1	B	32	ARG
1	B	41	GLU
1	B	49	GLU
1	B	52	ASP
1	B	59	LEU
1	B	61	VAL
1	B	96	LEU
1	B	101	VAL

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Mol	Chain	Res	Type
1	B	109	GLU
1	B	122	VAL
1	B	146	LEU
1	B	168	VAL
1	B	187	THR
1	B	206	PRO
1	B	209	ARG
1	B	225	LEU
1	B	227	ASP
1	B	248	THR
1	C	8	THR
1	C	10	ILE
1	C	38	VAL
1	C	40	ASP
1	C	41	GLU
1	C	66	ASP
1	C	75	ARG
1	C	95	PHE
1	C	98	THR
1	C	122	VAL
1	C	144	MET
1	C	168	VAL
1	C	173	ASP
1	C	174	ARG
1	C	202	TYR
1	C	206	PRO
1	C	207	MET
1	C	223	LYS
1	C	226	SER
1	C	230	SER
1	C	244	THR
1	C	245	THR
1	D	4	LEU
1	D	8	THR
1	D	9	VAL
1	D	10	ILE
1	D	32	ARG
1	D	35	LEU
1	D	41	GLU
1	D	61	VAL
1	D	101	VAL
1	D	102	GLU

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Mol	Chain	Res	Type
1	D	133	SER
1	D	163	SER
1	D	189	MET
1	D	190	THR
1	D	193	THR
1	D	206	PRO
1	D	223	LYS
1	D	225	LEU
1	D	240	ASP
1	D	244	THR
1	D	245	THR
1	D	255	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	68	GLN
1	A	87	ASN
1	A	178	ASN
1	A	204	ASN
1	B	87	ASN
1	B	178	ASN
1	B	255	GLN
1	C	2	ASN
1	C	201	ASN
1	D	57	GLN
1	D	68	GLN
1	D	178	ASN
1	D	255	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CBO	B	301	-	45,45,45	3.21	18 (40%)	76,76,76	2.48	24 (31%)
2	CBO	A	301	-	45,45,45	2.71	19 (42%)	76,76,76	1.80	23 (30%)
2	CBO	D	301	-	45,45,45	2.72	23 (51%)	76,76,76	2.95	21 (27%)
2	CBO	C	301	-	45,45,45	2.72	19 (42%)	76,76,76	2.78	22 (28%)

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
2	CBO	B	301	-	-	1/15/109/109	0/5/5/5
2	CBO	A	301	-	-	1/15/109/109	0/5/5/5
2	CBO	D	301	-	-	12/15/109/109	0/5/5/5
2	CBO	C	301	-	-	5/15/109/109	0/5/5/5

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CBO	C26-C8	10.06	1.74	1.54
2	B	301	CBO	C1-C10	9.35	1.70	1.54
2	C	301	CBO	C26-C8	8.55	1.71	1.54
2	B	301	CBO	C15-C14	7.36	1.66	1.54
2	D	301	CBO	C15-C14	7.25	1.66	1.54
2	A	301	CBO	C19-C10	6.98	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	CBO	C15-C14	6.97	1.65	1.54
2	D	301	CBO	C7-C8	6.82	1.66	1.54
2	D	301	CBO	C26-C8	6.54	1.67	1.54
2	A	301	CBO	C26-C8	6.40	1.67	1.54
2	C	301	CBO	C7-C8	6.33	1.66	1.54
2	B	301	CBO	C7-C8	6.20	1.65	1.54
2	B	301	CBO	C10-C9	5.90	1.65	1.56
2	A	301	CBO	C7-C8	5.79	1.65	1.54
2	A	301	CBO	C15-C14	5.24	1.63	1.54
2	A	301	CBO	C1-C10	-4.85	1.45	1.54
2	B	301	CBO	C17-C18	4.54	1.62	1.55
2	D	301	CBO	C8-C9	4.36	1.61	1.56
2	C	301	CBO	C8-C9	4.34	1.61	1.56
2	C	301	CBO	C6-C5	4.26	1.60	1.53
2	A	301	CBO	C10-C9	4.25	1.63	1.56
2	A	301	CBO	C8-C9	4.21	1.61	1.56
2	B	301	CBO	O3-C3	-4.18	1.39	1.46
2	A	301	CBO	C6-C5	4.04	1.60	1.53
2	B	301	CBO	C12-C13	3.96	1.39	1.34
2	A	301	CBO	C21-C33	3.93	1.61	1.53
2	D	301	CBO	C8-C14	3.80	1.65	1.58
2	D	301	CBO	C16-C17	3.77	1.60	1.54
2	C	301	CBO	C16-C17	3.63	1.60	1.54
2	B	301	CBO	C16-C17	3.49	1.60	1.54
2	D	301	CBO	C17-C18	3.30	1.60	1.55
2	D	301	CBO	O11-C11	3.25	1.27	1.22
2	C	301	CBO	O11-C11	3.20	1.27	1.22
2	D	301	CBO	C20-C18	3.19	1.60	1.54
2	B	301	CBO	C8-C9	3.18	1.60	1.56
2	C	301	CBO	C14-C13	-3.12	1.48	1.53
2	D	301	CBO	C12-C13	3.08	1.38	1.34
2	D	301	CBO	C24-C4	3.06	1.61	1.53
2	B	301	CBO	C6-C5	3.06	1.58	1.53
2	D	301	CBO	C10-C9	3.03	1.61	1.56
2	A	301	CBO	C17-C18	3.03	1.60	1.55
2	D	301	CBO	C6-C5	3.01	1.58	1.53
2	C	301	CBO	C22-C21	2.93	1.59	1.54
2	C	301	CBO	C24-C4	2.93	1.61	1.53
2	C	301	CBO	C20-C18	2.90	1.59	1.54
2	C	301	CBO	C17-C18	2.90	1.59	1.55
2	B	301	CBO	C10-C5	2.87	1.61	1.56
2	D	301	CBO	C22-C21	2.83	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CBO	C16-C17	2.79	1.59	1.54
2	C	301	CBO	C12-C13	2.78	1.37	1.34
2	A	301	CBO	C10-C5	2.72	1.60	1.56
2	B	301	CBO	C8-C14	2.66	1.63	1.58
2	D	301	CBO	O3-C3	-2.64	1.41	1.46
2	A	301	CBO	C24-C4	2.61	1.60	1.53
2	D	301	CBO	C20-C21	2.60	1.57	1.54
2	D	301	CBO	C14-C13	-2.50	1.49	1.53
2	D	301	CBO	C4-C3	2.46	1.59	1.54
2	A	301	CBO	O32-C32	2.46	1.30	1.22
2	A	301	CBO	C4-C5	2.43	1.60	1.56
2	C	301	CBO	C8-C14	2.41	1.62	1.58
2	C	301	CBO	C10-C9	2.41	1.60	1.56
2	B	301	CBO	O11-C11	2.39	1.26	1.22
2	B	301	CBO	C24-C4	2.39	1.59	1.53
2	A	301	CBO	C12-C11	-2.35	1.41	1.46
2	D	301	CBO	O32-C32	2.35	1.29	1.22
2	C	301	CBO	O34-C33	2.34	1.29	1.22
2	B	301	CBO	C4-C5	2.31	1.60	1.56
2	C	301	CBO	C23-C17	2.27	1.58	1.54
2	D	301	CBO	C27-C14	2.25	1.59	1.53
2	C	301	CBO	O29-C29	-2.23	1.15	1.22
2	B	301	CBO	C20-C18	2.21	1.58	1.54
2	C	301	CBO	C19-C10	-2.20	1.50	1.54
2	D	301	CBO	C9-C11	-2.17	1.50	1.52
2	A	301	CBO	C2-C3	2.15	1.56	1.51
2	A	301	CBO	C20-C18	2.13	1.58	1.54
2	A	301	CBO	O35-C33	2.12	1.38	1.30
2	D	301	CBO	C18-C13	2.09	1.56	1.52
2	D	301	CBO	C31-C30	2.04	1.58	1.52
2	B	301	CBO	O32-C32	2.02	1.28	1.22

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	CBO	C3-O3-C29	15.64	147.36	117.92
2	C	301	CBO	C1-C10-C9	-9.80	97.57	108.19
2	C	301	CBO	O3-C3-C2	8.85	123.65	108.48
2	C	301	CBO	C19-C10-C1	8.84	122.51	108.26
2	C	301	CBO	C26-C8-C14	8.12	119.53	109.97
2	B	301	CBO	C1-C10-C9	7.78	116.62	108.19
2	D	301	CBO	C1-C10-C5	7.47	117.17	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	CBO	C19-C10-C1	-7.34	96.43	108.26
2	B	301	CBO	C26-C8-C9	-7.32	102.80	110.39
2	D	301	CBO	O3-C3-C2	7.20	120.83	108.48
2	B	301	CBO	C19-C10-C1	-6.13	98.38	108.26
2	C	301	CBO	C14-C8-C9	-6.08	103.01	107.93
2	B	301	CBO	C26-C8-C14	5.90	116.92	109.97
2	B	301	CBO	C14-C8-C9	-5.62	103.37	107.93
2	A	301	CBO	C20-C18-C17	5.61	117.57	113.13
2	C	301	CBO	C19-C10-C5	-5.35	103.01	112.92
2	B	301	CBO	C1-C10-C5	5.31	114.52	108.02
2	D	301	CBO	C20-C18-C17	5.28	117.31	113.13
2	C	301	CBO	C26-C8-C9	-5.18	105.02	110.39
2	B	301	CBO	C2-C3-C4	5.10	121.87	114.39
2	C	301	CBO	C19-C10-C9	5.04	122.24	112.41
2	D	301	CBO	C17-C18-C13	-4.93	107.98	112.70
2	D	301	CBO	C26-C8-C14	4.78	115.59	109.97
2	D	301	CBO	C14-C8-C9	-4.69	104.13	107.93
2	B	301	CBO	C20-C18-C17	4.55	116.73	113.13
2	D	301	CBO	C2-C1-C10	4.47	120.45	112.78
2	C	301	CBO	C20-C18-C17	4.09	116.36	113.13
2	A	301	CBO	C3-O3-C29	3.70	124.89	117.92
2	A	301	CBO	O35-C33-C21	3.51	124.91	114.98
2	B	301	CBO	C8-C9-C10	3.48	120.64	118.10
2	B	301	CBO	O35-C33-C21	3.38	124.53	114.98
2	D	301	CBO	C6-C5-C4	3.34	118.13	114.11
2	A	301	CBO	C14-C8-C9	-3.32	105.24	107.93
2	D	301	CBO	C27-C14-C8	3.26	115.38	112.33
2	A	301	CBO	C27-C14-C8	3.25	115.37	112.33
2	A	301	CBO	C19-C10-C9	-3.23	106.11	112.41
2	B	301	CBO	C15-C14-C13	3.23	115.65	111.68
2	A	301	CBO	C10-C9-C11	3.13	118.19	115.50
2	C	301	CBO	C27-C14-C8	3.08	115.21	112.33
2	C	301	CBO	C7-C8-C9	3.06	113.08	109.77
2	D	301	CBO	C24-C4-C3	3.01	116.10	109.38
2	B	301	CBO	C20-C18-C13	-3.00	106.30	111.33
2	B	301	CBO	O33-C32-C31	2.95	123.49	114.03
2	D	301	CBO	C9-C10-C5	-2.93	103.04	106.47
2	A	301	CBO	O11-C11-C12	-2.91	116.48	121.50
2	C	301	CBO	O32-C32-C31	-2.90	113.76	123.08
2	C	301	CBO	C6-C5-C4	2.87	117.57	114.11
2	C	301	CBO	C17-C18-C13	-2.85	109.97	112.70
2	B	301	CBO	O32-C32-C31	-2.82	114.03	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	CBO	C34-C21-C22	2.78	114.08	109.76
2	A	301	CBO	O33-C32-C31	2.76	122.90	114.03
2	C	301	CBO	O33-C32-C31	2.75	122.86	114.03
2	A	301	CBO	C16-C15-C14	-2.74	109.67	113.83
2	A	301	CBO	C9-C10-C5	-2.73	103.28	106.47
2	A	301	CBO	C20-C18-C13	-2.72	106.78	111.33
2	C	301	CBO	C9-C10-C5	-2.69	103.33	106.47
2	D	301	CBO	O35-C33-C21	2.68	122.57	114.98
2	A	301	CBO	C1-C10-C5	2.63	111.25	108.02
2	D	301	CBO	O33-C32-C31	2.62	122.45	114.03
2	B	301	CBO	C7-C8-C9	2.60	112.58	109.77
2	D	301	CBO	O32-C32-C31	-2.59	114.76	123.08
2	B	301	CBO	C15-C14-C8	-2.54	107.46	110.51
2	A	301	CBO	C34-C21-C22	2.51	113.65	109.76
2	C	301	CBO	C27-C14-C13	-2.51	104.34	106.95
2	D	301	CBO	C1-C2-C3	2.50	115.44	110.63
2	C	301	CBO	C23-C22-C21	2.49	117.31	112.66
2	B	301	CBO	O3-C3-C4	-2.46	103.68	107.72
2	B	301	CBO	O35-C33-O34	-2.44	116.04	123.82
2	A	301	CBO	O32-C32-C31	-2.44	115.23	123.08
2	A	301	CBO	O35-C33-O34	-2.41	116.14	123.82
2	A	301	CBO	C26-C8-C7	2.41	111.95	107.84
2	D	301	CBO	C1-C10-C9	2.35	110.74	108.19
2	A	301	CBO	C19-C10-C5	2.34	117.27	112.92
2	C	301	CBO	C34-C21-C22	2.34	113.39	109.76
2	C	301	CBO	C10-C9-C11	2.33	117.50	115.50
2	B	301	CBO	C28-C17-C23	-2.30	104.99	108.94
2	A	301	CBO	C27-C14-C13	-2.30	104.56	106.95
2	A	301	CBO	C21-C20-C18	-2.28	110.22	113.55
2	A	301	CBO	C15-C14-C8	-2.28	107.78	110.51
2	B	301	CBO	C16-C17-C18	2.28	111.88	109.02
2	B	301	CBO	O3-C3-C2	-2.28	104.57	108.48
2	C	301	CBO	C20-C18-C13	-2.26	107.54	111.33
2	B	301	CBO	C16-C15-C14	2.23	117.20	113.83
2	B	301	CBO	C10-C9-C11	2.18	117.37	115.50
2	D	301	CBO	C26-C8-C9	-2.14	108.17	110.39
2	D	301	CBO	C16-C17-C18	2.08	111.63	109.02
2	D	301	CBO	C2-C3-C4	2.08	117.44	114.39
2	A	301	CBO	C8-C9-C10	2.05	119.60	118.10
2	A	301	CBO	C24-C4-C3	2.03	113.91	109.38
2	C	301	CBO	C16-C17-C18	2.03	111.56	109.02

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	CBO	C2-C3-O3-C29
2	D	301	CBO	C34-C21-C33-O35
2	D	301	CBO	C30-C29-O3-C3
2	D	301	CBO	O29-C29-O3-C3
2	D	301	CBO	C29-C30-C31-C32
2	D	301	CBO	C4-C3-O3-C29
2	A	301	CBO	C29-C30-C31-C32
2	D	301	CBO	C20-C21-C33-O35
2	C	301	CBO	C30-C29-O3-C3
2	C	301	CBO	O29-C29-O3-C3
2	D	301	CBO	C34-C21-C33-O34
2	D	301	CBO	C20-C21-C33-O34
2	C	301	CBO	C29-C30-C31-C32
2	C	301	CBO	C30-C31-C32-O33
2	B	301	CBO	C29-C30-C31-C32
2	C	301	CBO	C30-C31-C32-O32
2	D	301	CBO	C22-C21-C33-O35
2	D	301	CBO	C30-C31-C32-O33
2	D	301	CBO	C30-C31-C32-O32

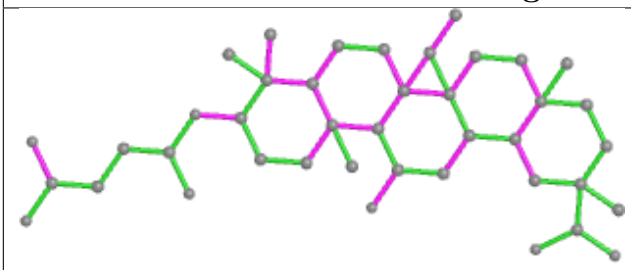
There are no ring outliers.

4 monomers are involved in 48 short contacts:

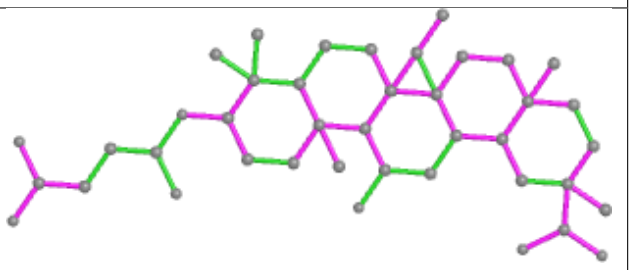
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CBO	7	0
2	A	301	CBO	11	0
2	D	301	CBO	20	0
2	C	301	CBO	10	0

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.

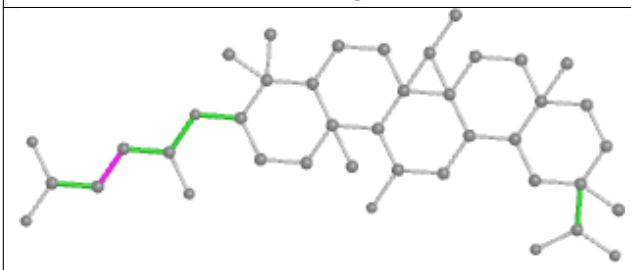
Ligand CBO B 301



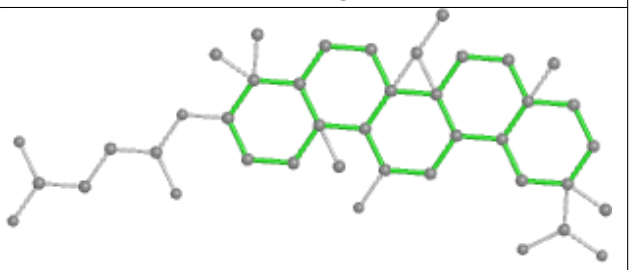
Bond lengths



Bond angles

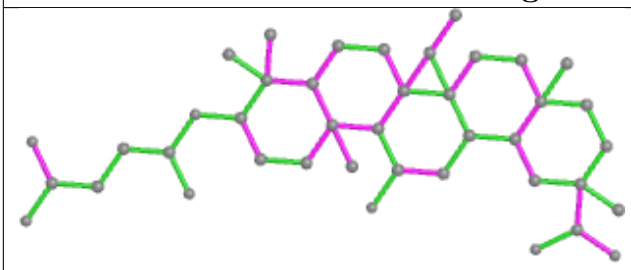


Torsions

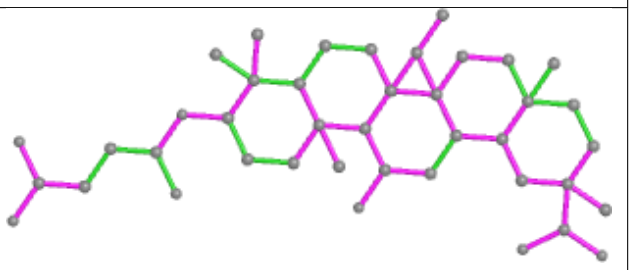


Rings

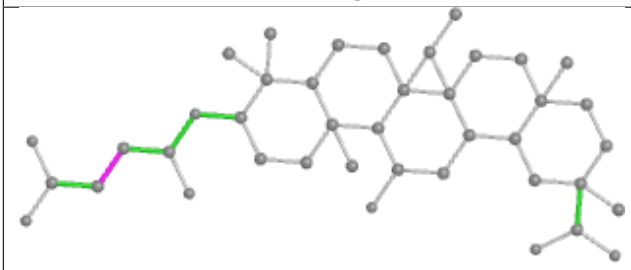
Ligand CBO A 301



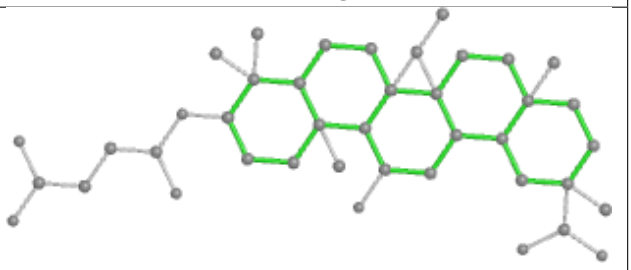
Bond lengths



Bond angles

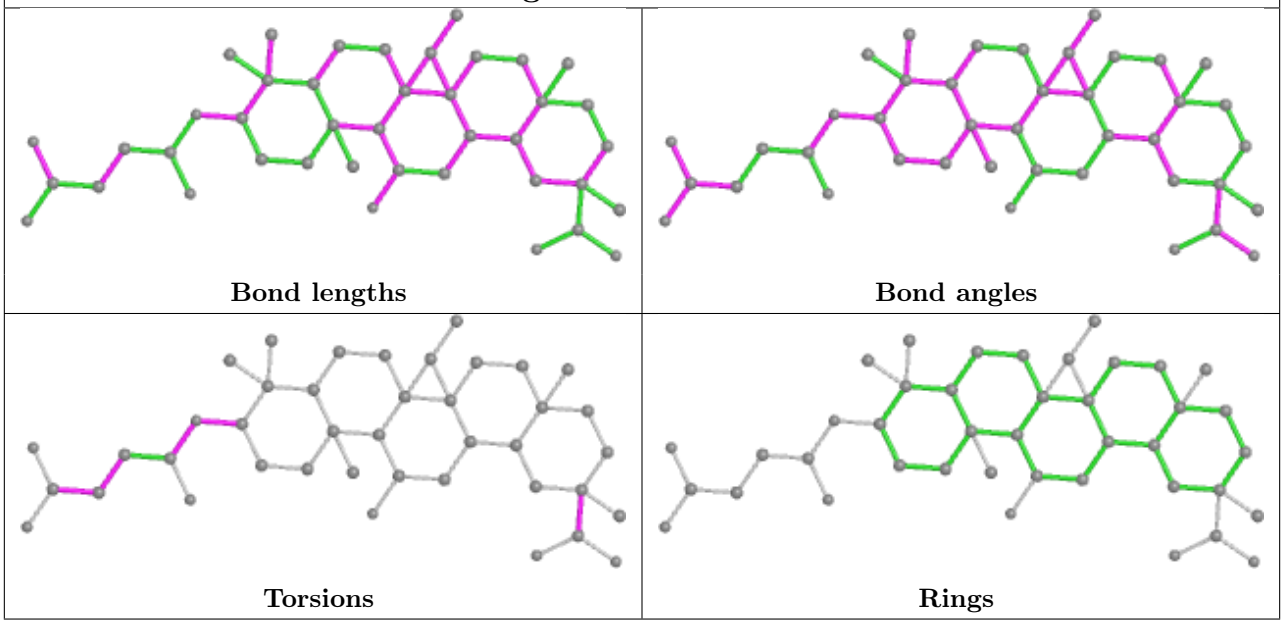


Torsions

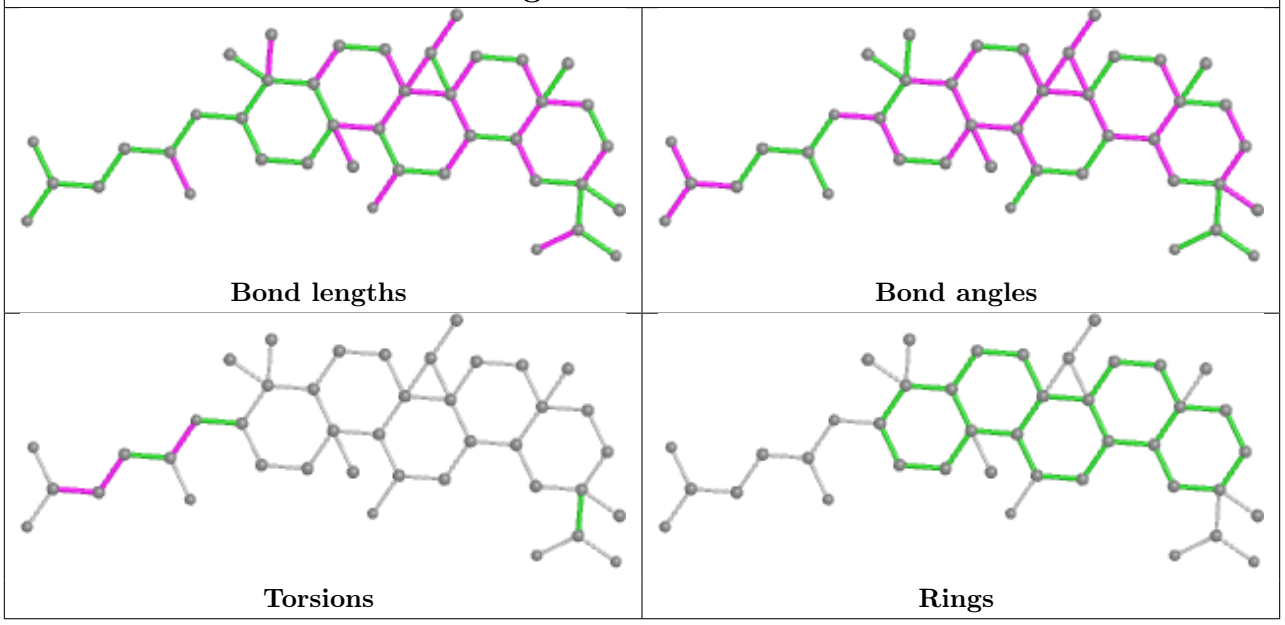


Rings

Ligand CBO D 301



Ligand CBO C 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.