Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:37 PM EDT

PDB ID	:	1EX4
Title	:	HIV-1 INTEGRASE CATALYTIC CORE AND C-TERMINAL DOMAIN
Authors	:	Chen, J.C.-H.; Krucinski, J.; Miercke, L.J.W.; Finer-Moore, J.S.; Tang, A.H.; Leavitt, A.D.; Stroud, R.M.
Deposited on	:	2000-04-28
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

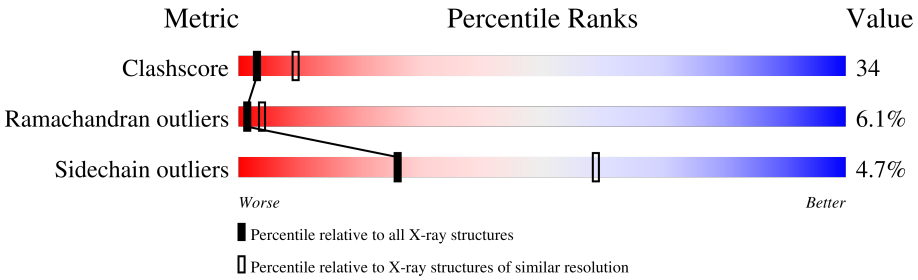
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	239	43% 41% 5% 11%
1	B	239	38% 42% . 15%

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
2	CPS	A	302	X	-	-	-
2	CPS	A	304	X	-	-	-
2	CPS	B	301	X	-	-	-
2	CPS	B	303	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3450 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.

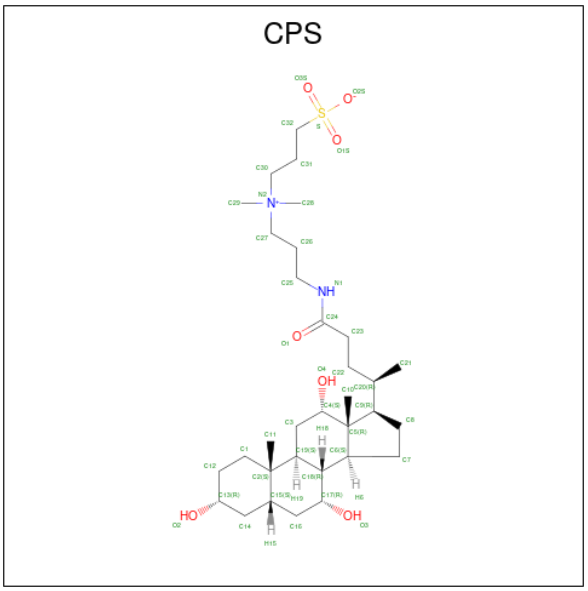
- Molecule 1 is a protein called INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1653	1046	299	304	4			
1	B	204	Total	C	N	O	S	0	0	0
			1601	1016	290	291	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLY	-	cloning artifact	UNP P04585
A	51	SER	-	cloning artifact	UNP P04585
A	56	SER	CYS	engineered mutation	UNP P04585
A	131	ASP	TRP	engineered mutation	UNP P04585
A	139	ASP	PHE	engineered mutation	UNP P04585
A	185	LYS	PHE	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585
B	50	GLY	-	cloning artifact	UNP P04585
B	51	SER	-	cloning artifact	UNP P04585
B	56	SER	CYS	engineered mutation	UNP P04585
B	131	ASP	TRP	engineered mutation	UNP P04585
B	139	ASP	PHE	engineered mutation	UNP P04585
B	185	LYS	PHE	engineered mutation	UNP P04585
B	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 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
2	A	1	Total C O 25 22 3	0	0
2	A	1	Total C O 25 22 3	0	0
2	B	1	Total C O 25 22 3	0	0
2	B	1	Total C N O S 42 32 2 7 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	0	0
3	B	30	Total O 30 30	0	0

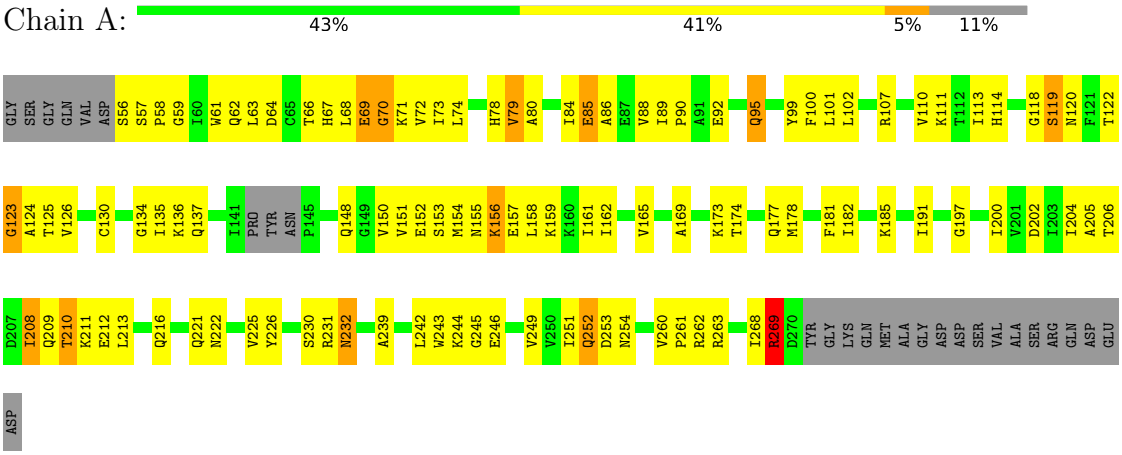
3 Residue-property plots (i)

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.

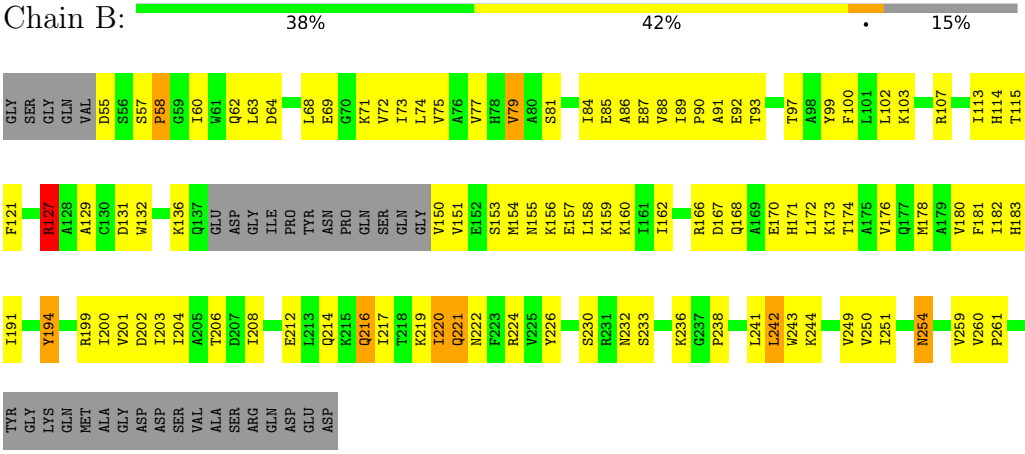
• Molecule 1: INTEGRASE

Chain A:



• Molecule 1: INTEGRASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 3 1 2	Depositor
Cell constants a, b, c, α, β, γ	103.99Å 103.99Å 101.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.26 – 2.80	Depositor
% Data completeness (in resolution range)	99.7 (28.26-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3450	wwPDB-VP
Average B, all atoms (Å^2)	72.0	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: CPS

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	0.36	0/1681	0.64	0/2267
1	B	0.35	0/1628	0.60	0/2195
All	All	0.36	0/3309	0.62	0/4462

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1653	0	1688	113	1
1	B	1601	0	1647	118	0
2	A	50	0	68	7	2
2	B	67	0	91	18	0
3	A	49	0	0	4	0
3	B	30	0	0	10	1
All	All	3450	0	3494	235	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 34.

All (235) 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:269:ARG:H	1:A:269:ARG:HD2	1.32	0.95
1:B:221:GLN:HE21	1:B:221:GLN:HA	1.30	0.95
1:A:177:GLN:HE21	1:A:177:GLN:HA	1.36	0.90
1:A:95:GLN:HE21	1:A:95:GLN:HA	1.37	0.88
1:A:177:GLN:HA	1:A:177:GLN:NE2	1.93	0.82
1:A:269:ARG:HD2	1:A:269:ARG:N	1.96	0.81
1:B:156:LYS:NZ	1:B:160:LYS:HE2	1.96	0.80
1:B:55:ASP:HB2	1:B:136:LYS:NZ	1.98	0.79
1:B:77:VAL:HG22	1:B:84:ILE:HG12	1.66	0.78
1:A:74:LEU:HG	1:A:89:ILE:HD13	1.64	0.78
1:B:156:LYS:HZ3	1:B:160:LYS:HE2	1.49	0.77
1:B:217:ILE:O	1:B:221:GLN:HG2	1.86	0.76
1:A:202:ASP:O	1:A:206:THR:HG23	1.85	0.75
1:B:158:LEU:O	1:B:162:ILE:HG13	1.87	0.75
1:B:242:LEU:O	2:B:303:CPS:H23	1.87	0.74
1:B:91:ALA:HB1	1:B:93:THR:HG23	1.70	0.73
1:B:250:VAL:HG22	1:B:259:VAL:HG22	1.69	0.73
1:B:156:LYS:HG2	1:B:160:LYS:HZ3	1.53	0.73
1:B:221:GLN:HE21	1:B:221:GLN:CA	2.03	0.72
1:B:69:GLU:HG3	1:B:172:LEU:HD22	1.72	0.71
1:A:84:ILE:HG22	1:A:85:GLU:H	1.56	0.70
1:B:84:ILE:HD11	1:B:154:MET:SD	2.32	0.70
1:B:127:ARG:HH21	1:B:131:ASP:CG	1.95	0.70
1:A:252:GLN:HG3	1:A:252:GLN:O	1.90	0.70
1:A:205:ALA:HB2	1:B:201:VAL:HG12	1.73	0.70
1:B:55:ASP:HB2	1:B:136:LYS:HZ2	1.55	0.70
1:B:127:ARG:HE	1:B:131:ASP:HB2	1.56	0.69
2:B:303:CPS:H29A	3:B:318:HOH:O	1.90	0.69
1:A:84:ILE:HG22	1:A:85:GLU:N	2.09	0.68
1:B:62:GLN:HE21	1:B:151:VAL:HB	1.59	0.68
1:A:158:LEU:O	1:A:162:ILE:HG13	1.96	0.66
1:B:221:GLN:HA	1:B:221:GLN:NE2	2.08	0.65
2:B:303:CPS:H12	3:B:332:HOH:O	1.97	0.64
1:A:206:THR:O	1:A:210:THR:HB	1.98	0.64
1:B:69:GLU:HB3	1:B:71:LYS:NZ	2.12	0.64
1:A:152:GLU:C	1:A:154:MET:H	2.00	0.64
1:A:95:GLN:HA	1:A:95:GLN:NE2	2.11	0.63
1:B:153:SER:O	1:B:157:GLU:HG2	1.98	0.63
1:B:233:SER:HB3	3:B:310:HOH:O	1.98	0.63
1:A:205:ALA:O	1:A:209:GLN:HG2	1.99	0.62
1:A:74:LEU:HD13	1:A:100:PHE:CD2	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:VAL:HB	3:B:327:HOH:O	1.99	0.62
1:B:181:PHE:O	1:B:185:LYS:HG2	1.99	0.62
1:B:202:ASP:O	1:B:206:THR:HG23	1.99	0.62
1:A:57:SER:N	1:A:58:PRO:HD2	2.15	0.62
1:B:77:VAL:HG23	1:B:84:ILE:HG23	1.80	0.62
1:A:59:GLY:HA3	1:A:111:LYS:HD2	1.82	0.62
1:A:216:GLN:OE1	2:A:304:CPS:H21	2.01	0.60
1:B:217:ILE:HG12	2:B:303:CPS:C21	2.31	0.60
1:A:74:LEU:HD12	1:A:89:ILE:HG21	1.83	0.60
1:B:230:SER:C	1:B:232:ASN:H	2.06	0.59
1:A:269:ARG:HH12	2:A:302:CPS:H7	1.67	0.59
2:A:302:CPS:O4	2:A:302:CPS:H21A	2.03	0.59
1:B:84:ILE:HG22	1:B:85:GLU:H	1.67	0.59
1:B:243:TRP:CD1	2:B:303:CPS:H4	2.38	0.59
1:A:249:VAL:HG12	1:A:251:ILE:HG23	1.84	0.59
1:A:254:ASN:HB2	3:A:349:HOH:O	2.02	0.59
1:A:191:ILE:O	1:A:191:ILE:HG23	2.02	0.58
1:A:84:ILE:HD11	1:A:154:MET:SD	2.43	0.58
1:A:63:LEU:HD11	1:A:113:ILE:HD12	1.84	0.58
1:A:268:ILE:HD11	2:A:302:CPS:O3	2.03	0.58
1:A:191:ILE:HD13	1:B:219:LYS:HD2	1.86	0.57
1:B:244:LYS:HZ3	2:B:303:CPS:H32A	1.69	0.57
1:A:152:GLU:HA	1:A:155:ASN:ND2	2.19	0.57
1:B:158:LEU:HG	1:B:162:ILE:HD11	1.85	0.57
1:A:191:ILE:HG21	1:B:219:LYS:HD2	1.87	0.57
1:B:156:LYS:HG2	1:B:160:LYS:NZ	2.19	0.57
1:B:199:ARG:O	1:B:203:ILE:HG13	2.05	0.57
1:A:155:ASN:O	1:A:159:LYS:HG3	2.04	0.56
1:A:136:LYS:HG2	1:A:137:GLN:N	2.20	0.56
1:A:67:HIS:HD2	1:A:72:VAL:HG22	1.70	0.56
1:A:61:TRP:CZ3	1:A:78:HIS:HB2	2.41	0.56
1:A:99:TYR:OH	1:B:173:LYS:HB2	2.05	0.56
1:B:167:ASP:O	1:B:168:GLN:HG3	2.06	0.56
1:B:243:TRP:HB2	2:B:303:CPS:C10	2.36	0.56
1:A:177:GLN:NE2	1:A:177:GLN:CA	2.63	0.55
1:A:72:VAL:HG12	1:A:73:ILE:N	2.21	0.55
1:B:57:SER:O	1:B:60:ILE:HG13	2.06	0.55
1:B:172:LEU:O	1:B:176:VAL:HG23	2.07	0.55
1:B:173:LYS:HG3	1:B:174:THR:H	1.71	0.55
1:B:176:VAL:O	1:B:180:VAL:HG23	2.06	0.55
1:B:173:LYS:HG3	1:B:174:THR:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:HIS:CE1	1:A:80:ALA:HB3	2.42	0.55
1:A:269:ARG:H	1:A:269:ARG:CD	2.03	0.55
1:B:84:ILE:HG22	1:B:85:GLU:N	2.21	0.54
1:B:214:GLN:HG2	3:B:319:HOH:O	2.08	0.54
1:A:68:LEU:HG	1:A:69:GLU:HG2	1.89	0.54
1:A:178:MET:O	1:A:182:ILE:HG13	2.08	0.54
1:B:217:ILE:O	1:B:220:ILE:HG22	2.08	0.53
2:B:303:CPS:H28B	3:B:318:HOH:O	2.09	0.53
1:A:56:SER:C	1:A:58:PRO:HD2	2.28	0.53
1:B:62:GLN:HG2	1:B:114:HIS:HB2	1.90	0.53
1:A:239:ALA:CB	1:A:251:ILE:HD12	2.39	0.53
1:B:167:ASP:C	1:B:168:GLN:HG3	2.29	0.53
1:B:178:MET:O	1:B:182:ILE:HG13	2.09	0.53
1:A:72:VAL:HG21	1:A:92:GLU:OE1	2.09	0.53
1:B:200:ILE:HG23	1:B:201:VAL:N	2.24	0.53
1:A:152:GLU:C	1:A:154:MET:N	2.63	0.53
1:A:66:THR:HG21	1:A:155:ASN:HB3	1.90	0.52
1:B:194:TYR:HA	3:B:321:HOH:O	2.09	0.52
1:B:156:LYS:HZ2	1:B:160:LYS:HE2	1.75	0.52
1:A:68:LEU:O	1:A:70:GLY:N	2.43	0.52
1:A:113:ILE:O	1:A:114:HIS:HD2	1.93	0.52
1:B:261:PRO:HD2	1:B:264:LYS:HD2	1.91	0.52
1:A:244:LYS:HE3	1:A:262:ARG:NH2	2.25	0.52
1:A:67:HIS:CD2	1:A:72:VAL:HG22	2.44	0.51
1:A:231:ARG:HA	1:A:231:ARG:NE	2.26	0.51
1:B:69:GLU:HB3	1:B:71:LYS:HZ1	1.74	0.51
1:A:57:SER:N	1:A:58:PRO:CD	2.73	0.51
1:A:62:GLN:HG2	1:A:114:HIS:HB2	1.93	0.51
1:B:182:ILE:O	1:B:186:LYS:HB2	2.11	0.51
1:B:73:ILE:HG23	1:B:87:GLU:O	2.10	0.50
1:B:183:HIS:HA	1:B:186:LYS:HE2	1.94	0.50
1:A:204:ILE:O	1:A:208:ILE:HG13	2.11	0.50
1:B:74:LEU:HD12	1:B:100:PHE:CE1	2.47	0.50
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.76	0.50
1:B:97:THR:O	1:B:100:PHE:HB3	2.12	0.50
1:A:211:LYS:C	1:A:213:LEU:H	2.15	0.50
2:B:303:CPS:H4	2:B:303:CPS:H23A	1.94	0.49
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.75	0.49
1:B:242:LEU:O	2:B:303:CPS:H10B	2.12	0.49
2:A:304:CPS:H20	2:A:304:CPS:O4	2.13	0.49
1:B:55:ASP:N	1:B:136:LYS:HD3	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLY:HA3	1:A:111:LYS:CD	2.43	0.48
1:A:113:ILE:CG1	1:A:135:ILE:HG21	2.43	0.48
1:A:118:GLY:O	1:A:120:ASN:N	2.46	0.48
1:B:81:SER:OG	1:B:200:ILE:HB	2.12	0.48
1:A:157:GLU:O	1:A:161:ILE:HG13	2.13	0.48
1:B:150:VAL:HG12	1:B:153:SER:HB3	1.96	0.48
1:A:63:LEU:CD1	1:A:113:ILE:HD12	2.44	0.48
1:A:74:LEU:O	1:A:86:ALA:HA	2.13	0.48
1:A:63:LEU:HD11	1:A:101:LEU:HD13	1.96	0.48
1:A:113:ILE:HG12	1:A:135:ILE:HG21	1.95	0.48
1:A:61:TRP:CH2	1:A:78:HIS:HB2	2.49	0.48
1:B:72:VAL:HG13	1:B:89:ILE:HG13	1.95	0.48
1:B:116:ASP:O	1:B:118:GLY:N	2.40	0.48
1:B:243:TRP:HA	2:B:303:CPS:HN1	1.79	0.47
1:A:153:SER:O	1:A:156:LYS:HE3	2.14	0.47
1:B:91:ALA:C	1:B:93:THR:H	2.18	0.47
1:A:72:VAL:HG12	1:A:73:ILE:H	1.78	0.47
1:B:74:LEU:HD12	1:B:100:PHE:CZ	2.50	0.47
1:A:107:ARG:HD3	3:B:320:HOH:O	2.15	0.47
1:B:86:ALA:O	1:B:87:GLU:HG3	2.14	0.47
1:A:269:ARG:N	1:A:269:ARG:CD	2.68	0.47
1:B:92:GLU:O	1:B:92:GLU:HG2	2.15	0.47
1:B:268:ILE:O	1:B:268:ILE:HG13	2.15	0.47
2:B:303:CPS:H10B	2:B:303:CPS:H20	1.75	0.47
1:B:63:LEU:HA	1:B:75:VAL:O	2.15	0.47
1:B:244:LYS:NZ	2:B:303:CPS:C32	2.78	0.47
1:A:58:PRO:HG2	1:A:111:LYS:HZ2	1.80	0.46
1:B:92:GLU:O	1:B:120:ASN:HB3	2.15	0.46
1:B:224:ARG:HB3	1:B:238:PRO:HB2	1.96	0.46
1:B:115:THR:HB	1:B:121:PHE:HB3	1.96	0.46
1:B:107:ARG:HD3	3:B:320:HOH:O	2.15	0.46
1:A:84:ILE:CG2	1:A:85:GLU:N	2.78	0.46
1:A:231:ARG:HG2	3:A:351:HOH:O	2.14	0.46
1:A:73:ILE:HG22	1:A:88:VAL:HA	1.98	0.46
1:B:244:LYS:HZ3	2:B:303:CPS:C32	2.28	0.46
1:B:171:HIS:CB	1:B:173:LYS:HG2	2.46	0.46
1:A:102:LEU:HD21	1:B:178:MET:HG3	1.98	0.45
1:A:173:LYS:HG3	1:A:174:THR:H	1.81	0.45
1:B:62:GLN:HE22	1:B:151:VAL:H	1.64	0.45
1:B:226:TYR:HA	1:B:236:LYS:O	2.16	0.45
1:A:231:ARG:O	1:A:232:ASN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:THR:HG22	1:A:122:THR:O	2.16	0.45
1:A:118:GLY:O	1:A:119:SER:C	2.55	0.45
1:A:263:ARG:HD3	3:A:309:HOH:O	2.16	0.45
1:A:73:ILE:HG22	1:A:88:VAL:HG22	1.98	0.45
1:B:72:VAL:HG11	1:B:92:GLU:HB2	1.98	0.45
1:A:124:ALA:C	1:A:126:VAL:H	2.20	0.44
1:A:152:GLU:HA	1:A:155:ASN:HD22	1.80	0.44
1:B:58:PRO:HA	3:B:324:HOH:O	2.17	0.44
1:B:99:TYR:CE2	1:B:103:LYS:HE3	2.53	0.44
1:A:71:LYS:HD2	1:A:71:LYS:HA	1.59	0.44
1:B:88:VAL:CG2	1:B:176:VAL:HG21	2.48	0.44
1:A:181:PHE:O	1:A:185:LYS:HG2	2.17	0.44
1:B:64:ASP:OD2	1:B:155:ASN:OD1	2.36	0.44
1:B:117:ASN:O	1:B:118:GLY:C	2.56	0.44
1:B:129:ALA:O	1:B:132:TRP:N	2.50	0.44
1:B:243:TRP:HB2	2:B:303:CPS:H10A	1.99	0.44
1:B:244:LYS:NZ	2:B:303:CPS:H32	2.33	0.44
1:A:165:VAL:HB	1:A:178:MET:CE	2.48	0.43
1:A:107:ARG:HG3	1:A:107:ARG:NH1	2.33	0.43
1:A:169:ALA:HB1	1:A:174:THR:HB	1.99	0.43
1:A:181:PHE:CD1	1:A:181:PHE:C	2.92	0.43
1:B:230:SER:C	1:B:232:ASN:N	2.72	0.43
1:A:191:ILE:HD13	1:B:219:LYS:CD	2.48	0.43
1:A:225:VAL:HG12	1:A:226:TYR:N	2.34	0.43
1:B:204:ILE:O	1:B:208:ILE:HG13	2.18	0.43
1:B:212:GLU:OE1	1:B:216:GLN:OE1	2.36	0.43
1:B:194:TYR:CD1	1:B:194:TYR:N	2.87	0.43
1:B:212:GLU:O	1:B:216:GLN:HB2	2.19	0.43
1:A:211:LYS:O	1:A:213:LEU:N	2.50	0.42
2:A:302:CPS:H10B	2:A:302:CPS:H20	1.91	0.42
1:B:127:ARG:NE	1:B:131:ASP:HB2	2.31	0.42
1:A:84:ILE:CG2	1:A:85:GLU:H	2.27	0.42
1:A:151:VAL:O	1:A:154:MET:HB3	2.19	0.42
1:B:74:LEU:HD13	1:B:75:VAL:N	2.35	0.42
1:A:153:SER:HA	1:A:156:LYS:HD2	2.02	0.42
1:A:125:THR:HG21	3:A:333:HOH:O	2.20	0.42
1:A:122:THR:O	1:A:123:GLY:O	2.38	0.42
1:A:221:GLN:NE2	1:A:252:GLN:HG2	2.35	0.42
1:A:260:VAL:HG12	1:A:261:PRO:O	2.20	0.42
1:B:156:LYS:CG	1:B:160:LYS:NZ	2.83	0.42
1:A:243:TRP:CH2	1:A:245:GLY:HA3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG13	1:A:150:VAL:HG11	2.02	0.41
1:A:156:LYS:HD3	1:A:157:GLU:N	2.34	0.41
1:B:221:GLN:NE2	1:B:241:LEU:O	2.53	0.41
1:A:78:HIS:HE1	1:A:80:ALA:HB3	1.84	0.41
1:B:63:LEU:HD12	1:B:113:ILE:HD12	2.02	0.41
1:B:69:GLU:CG	1:B:172:LEU:HD22	2.46	0.41
1:B:150:VAL:HG12	1:B:150:VAL:O	2.19	0.41
1:B:156:LYS:O	1:B:160:LYS:HG2	2.20	0.41
1:B:243:TRP:CG	2:B:303:CPS:H3A	2.55	0.41
1:B:68:LEU:HD13	1:B:159:LYS:HE3	2.02	0.41
1:B:249:VAL:HG12	1:B:251:ILE:HG23	2.02	0.41
1:A:111:LYS:O	1:A:135:ILE:HA	2.21	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.85	0.41
1:B:241:LEU:CD1	1:B:249:VAL:HG13	2.50	0.41
1:A:130:CYS:HB3	1:A:135:ILE:HB	2.02	0.41
1:B:107:ARG:HG3	1:B:107:ARG:NH1	2.35	0.41
1:B:171:HIS:HB2	1:B:173:LYS:HG2	2.03	0.41
1:A:61:TRP:CD1	1:A:110:VAL:HG13	2.56	0.41
1:A:71:LYS:HG3	1:A:72:VAL:H	1.86	0.41
2:A:302:CPS:H7	2:A:302:CPS:O3	2.20	0.41
1:B:62:GLN:NE2	1:B:151:VAL:H	2.17	0.41
2:B:303:CPS:H1A	2:B:303:CPS:H3	1.86	0.41
1:A:66:THR:O	1:A:72:VAL:HG13	2.21	0.41
1:A:230:SER:O	1:A:231:ARG:HB2	2.21	0.40
1:A:74:LEU:HD12	1:A:89:ILE:CG2	2.50	0.40
1:A:197:GLY:O	1:A:200:ILE:HG22	2.22	0.40
1:B:260:VAL:CG2	1:B:264:LYS:HB2	2.51	0.40
1:A:136:LYS:CG	1:A:137:GLN:N	2.83	0.40
1:B:219:LYS:O	1:B:222:ASN:HB2	2.21	0.40
1:B:242:LEU:HD12	1:B:242:LEU:HA	1.88	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:216:GLN:OE1	2:A:304:CPS:O2[6_565]	2.15	0.05
2:A:302:CPS:C16	3:B:315:HOH:O[3_565]	2.16	0.04

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	208/239 (87%)	167 (80%)	27 (13%)	14 (7%)	1	3
1	B	200/239 (84%)	165 (82%)	24 (12%)	11 (6%)	2	5
All	All	408/478 (85%)	332 (81%)	51 (12%)	25 (6%)	1	4

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	B	79	VAL
1	A	119	SER
1	A	123	GLY
1	A	212	GLU
1	B	90	PRO
1	B	117	ASN
1	B	118	GLY
1	B	127	ARG
1	B	254	ASN
1	A	85	GLU
1	A	90	PRO
1	A	148	GLN
1	A	232	ASN
1	A	269	ARG
1	B	170	GLU
1	B	166	ARG
1	B	191	ILE
1	A	79	VAL
1	A	134	GLY
1	A	253	ASP
1	A	70	GLY
1	A	208	ILE
1	B	58	PRO
1	B	190	GLY

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	174/196 (89%)	166 (95%)	8 (5%)	27 60
1	B	169/196 (86%)	161 (95%)	8 (5%)	26 59
All	All	343/392 (88%)	327 (95%)	16 (5%)	26 59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	95	GLN
1	A	156	LYS
1	A	210	THR
1	A	222	ASN
1	A	246	GLU
1	A	252	GLN
1	A	269	ARG
1	B	102	LEU
1	B	127	ARG
1	B	194	TYR
1	B	216	GLN
1	B	220	ILE
1	B	221	GLN
1	B	242	LEU
1	B	254	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	95	GLN
1	A	114	HIS
1	A	146	GLN
1	A	148	GLN
1	A	155	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	GLN
1	A	209	GLN
1	A	214	GLN
1	A	221	GLN
1	A	222	ASN
1	B	62	GLN
1	B	95	GLN
1	B	114	HIS
1	B	155	ASN
1	B	168	GLN
1	B	183	HIS
1	B	214	GLN
1	B	216	GLN
1	B	221	GLN
1	B	222	ASN
1	B	254	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CPS	A	302	-	28,28,45	0.91	1 (3%)	46,46,70	4.42	26 (56%)
2	CPS	B	301	-	28,28,45	0.82	1 (3%)	46,46,70	3.73	23 (50%)
2	CPS	B	303	-	45,45,45	1.28	4 (8%)	69,70,70	3.74	26 (37%)
2	CPS	A	304	-	28,28,45	0.92	2 (7%)	46,46,70	3.98	21 (45%)

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	CPS	A	302	-	3/3/11/15	4/4/69/90	0/4/4/4
2	CPS	B	301	-	3/3/11/15	0/4/69/90	0/4/4/4
2	CPS	B	303	-	4/4/14/15	10/25/90/90	0/4/4/4
2	CPS	A	304	-	3/3/11/15	0/4/69/90	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	CPS	O3S-S	5.55	1.61	1.45
2	B	303	CPS	C2-C19	-2.77	1.51	1.56
2	B	303	CPS	C24-N1	2.76	1.39	1.33
2	B	301	CPS	C2-C19	-2.74	1.51	1.56
2	A	304	CPS	C2-C19	-2.59	1.51	1.56
2	B	303	CPS	C3-C19	-2.39	1.49	1.53
2	A	302	CPS	C2-C19	-2.37	1.51	1.56
2	A	304	CPS	C3-C19	-2.17	1.50	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	303	CPS	C2-C19-C18	16.56	129.60	111.82
2	A	304	CPS	C3-C19-C2	12.46	126.58	113.73
2	A	304	CPS	C2-C19-C18	11.59	124.26	111.82
2	A	302	CPS	C6-C5-C4	11.30	117.92	107.40
2	B	301	CPS	C3-C19-C2	11.12	125.20	113.73
2	B	303	CPS	C9-C5-C4	-11.02	107.61	117.67
2	B	301	CPS	C2-C19-C18	10.76	123.37	111.82
2	A	302	CPS	C3-C19-C2	10.43	124.48	113.73
2	A	302	CPS	C15-C16-C17	-9.89	103.55	114.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	304	CPS	C6-C5-C4	9.88	116.60	107.40
2	A	302	CPS	C2-C19-C18	9.72	122.26	111.82
2	A	302	CPS	C9-C5-C4	-9.10	109.36	117.67
2	B	303	CPS	C10-C5-C4	9.00	118.23	109.07
2	B	301	CPS	C6-C5-C4	8.71	115.51	107.40
2	B	303	CPS	C10-C5-C6	-8.57	97.79	111.21
2	A	304	CPS	C8-C9-C5	7.80	111.20	103.55
2	B	303	CPS	C6-C5-C4	7.16	114.06	107.40
2	B	303	CPS	C5-C9-C20	-6.64	111.57	119.50
2	A	302	CPS	C8-C9-C5	6.51	109.94	103.55
2	B	301	CPS	C3-C4-C5	6.33	117.74	111.24
2	A	302	CPS	C10-C5-C6	-6.28	101.38	111.21
2	B	303	CPS	C9-C5-C6	6.15	106.29	100.09
2	A	304	CPS	C9-C5-C4	-5.90	112.28	117.67
2	B	301	CPS	C9-C5-C4	-5.84	112.33	117.67
2	B	303	CPS	C3-C19-C18	5.82	119.39	110.88
2	A	302	CPS	C19-C18-C17	-5.69	105.07	111.88
2	A	302	CPS	C19-C2-C15	5.54	116.37	108.58
2	B	303	CPS	C8-C9-C20	5.31	120.37	112.15
2	B	301	CPS	C16-C15-C14	-5.30	105.09	111.19
2	A	302	CPS	C10-C5-C4	5.19	114.35	109.07
2	A	302	CPS	C11-C2-C19	-5.02	104.26	111.18
2	A	302	CPS	C6-C18-C17	-5.01	105.17	111.81
2	B	303	CPS	C19-C18-C17	-4.98	105.92	111.88
2	B	301	CPS	C19-C18-C17	4.88	117.71	111.88
2	B	303	CPS	C16-C15-C14	-4.83	105.63	111.19
2	A	302	CPS	C16-C17-C18	-4.79	106.37	111.48
2	A	302	CPS	C3-C4-C5	4.78	116.15	111.24
2	B	301	CPS	C11-C2-C19	-4.74	104.66	111.18
2	A	304	CPS	C3-C19-C18	-4.66	104.06	110.88
2	B	301	CPS	C10-C5-C6	-4.61	104.00	111.21
2	A	304	CPS	C19-C2-C15	4.58	115.01	108.58
2	A	304	CPS	C16-C15-C14	-4.58	105.92	111.19
2	A	304	CPS	C19-C3-C4	-4.40	108.49	114.30
2	A	304	CPS	C3-C4-C5	4.33	115.69	111.24
2	B	301	CPS	C19-C2-C15	4.27	114.58	108.58
2	A	304	CPS	C1-C2-C15	4.26	114.07	107.77
2	A	304	CPS	C15-C16-C17	-4.25	109.77	114.46
2	B	301	CPS	C7-C6-C18	-4.07	112.64	118.33
2	A	304	CPS	C5-C6-C18	-3.91	109.74	114.74
2	A	304	CPS	C10-C5-C6	-3.90	105.10	111.21
2	A	304	CPS	C11-C2-C19	-3.90	105.81	111.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	303	CPS	C25-N1-C24	3.84	129.97	122.84
2	B	301	CPS	C5-C9-C20	-3.80	114.95	119.49
2	A	302	CPS	C7-C6-C5	3.73	107.21	103.55
2	B	301	CPS	C6-C18-C17	3.70	116.72	111.81
2	B	303	CPS	C22-C20-C9	3.70	117.92	110.28
2	A	304	CPS	C14-C13-C12	3.69	114.96	110.55
2	A	302	CPS	C11-C2-C15	-3.64	104.18	110.36
2	B	303	CPS	C14-C13-C12	3.58	114.82	110.55
2	B	301	CPS	C3-C19-C18	-3.56	105.67	110.88
2	A	302	CPS	C1-C12-C13	3.50	114.96	110.47
2	B	303	CPS	C1-C2-C19	-3.37	106.06	111.35
2	A	302	CPS	C14-C15-C2	3.35	116.22	112.66
2	B	303	CPS	C22-C23-C24	3.28	120.36	113.04
2	B	303	CPS	C8-C9-C5	3.26	106.75	103.55
2	B	301	CPS	C9-C5-C6	3.14	103.26	100.09
2	B	303	CPS	C19-C2-C15	3.10	112.93	108.58
2	B	301	CPS	C1-C2-C15	3.09	112.34	107.77
2	B	301	CPS	C8-C9-C5	3.06	106.55	103.55
2	B	301	CPS	C5-C6-C18	-2.91	111.02	114.74
2	A	302	CPS	O4-C4-C5	-2.89	106.14	111.03
2	A	302	CPS	C1-C2-C15	2.74	111.83	107.77
2	B	303	CPS	C3-C19-C2	-2.68	110.96	113.73
2	A	302	CPS	C14-C13-C12	2.67	113.74	110.55
2	B	301	CPS	C1-C12-C13	2.66	113.89	110.47
2	B	301	CPS	C11-C2-C15	-2.64	105.88	110.36
2	A	302	CPS	C19-C3-C4	-2.57	110.90	114.30
2	B	303	CPS	C7-C6-C18	2.55	121.90	118.33
2	B	303	CPS	C11-C2-C19	-2.46	107.79	111.18
2	B	301	CPS	C15-C16-C17	-2.43	111.78	114.46
2	B	303	CPS	C1-C2-C15	2.36	111.26	107.77
2	B	303	CPS	O2S-S-O1S	2.35	117.02	111.27
2	A	302	CPS	C16-C15-C14	-2.35	108.49	111.19
2	A	302	CPS	C5-C6-C18	2.35	117.73	114.74
2	A	302	CPS	C5-C9-C20	-2.32	116.72	119.49
2	A	304	CPS	C11-C2-C1	-2.28	104.59	108.26
2	A	304	CPS	C11-C2-C15	-2.26	106.53	110.36
2	A	304	CPS	C8-C9-C20	2.22	118.31	113.66
2	A	304	CPS	C16-C17-C18	-2.21	109.12	111.48
2	B	303	CPS	C29-N2-C27	2.20	115.06	109.46
2	B	301	CPS	C8-C7-C6	-2.20	100.78	105.13
2	B	303	CPS	C15-C16-C17	-2.12	112.12	114.46
2	A	304	CPS	C6-C18-C17	2.10	114.59	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	303	CPS	C5-C6-C18	2.04	117.35	114.74
2	A	302	CPS	C19-C18-C6	2.01	112.47	109.71
2	B	301	CPS	C14-C13-C12	2.00	112.94	110.55

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	302	CPS	C18
2	A	302	CPS	C6
2	A	302	CPS	C19
2	A	304	CPS	C18
2	A	304	CPS	C6
2	A	304	CPS	C19
2	B	301	CPS	C18
2	B	301	CPS	C6
2	B	301	CPS	C19
2	B	303	CPS	C18
2	B	303	CPS	C19
2	B	303	CPS	C20
2	B	303	CPS	C6

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	CPS	C21-C20-C9-C5
2	A	302	CPS	C22-C20-C9-C5
2	A	302	CPS	C21-C20-C9-C8
2	A	302	CPS	C22-C20-C9-C8
2	B	303	CPS	C21-C20-C9-C8
2	B	303	CPS	C22-C20-C9-C8
2	B	303	CPS	C26-C27-N2-C28
2	B	303	CPS	C26-C27-N2-C29
2	B	303	CPS	C26-C27-N2-C30
2	B	303	CPS	C22-C20-C9-C5
2	B	303	CPS	C21-C20-C22-C23
2	B	303	CPS	C9-C20-C22-C23
2	B	303	CPS	C21-C20-C9-C5
2	B	303	CPS	C26-C25-N1-C24

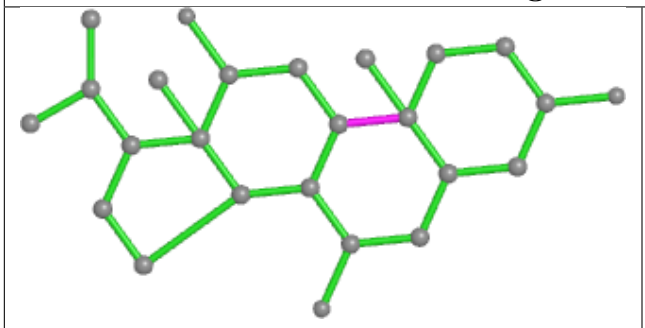
There are no ring outliers.

3 monomers are involved in 27 short contacts:

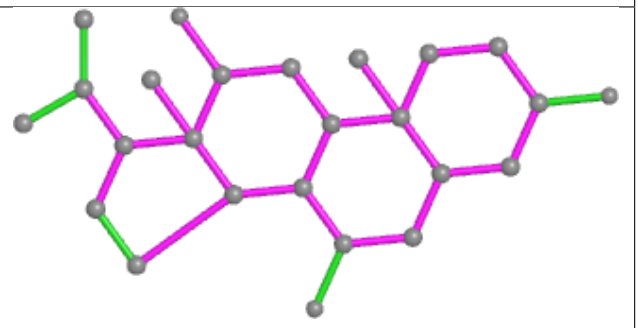
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	CPS	5	1
2	B	303	CPS	18	0
2	A	304	CPS	2	1

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.

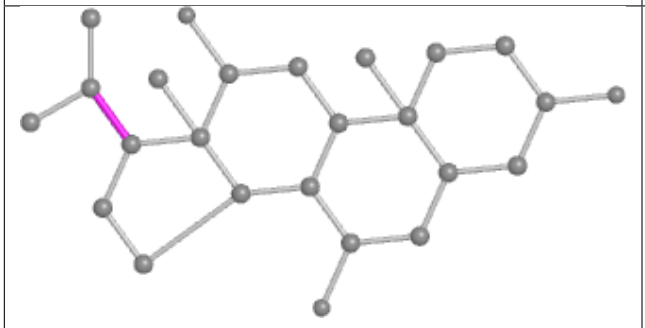
Ligand CPS A 302



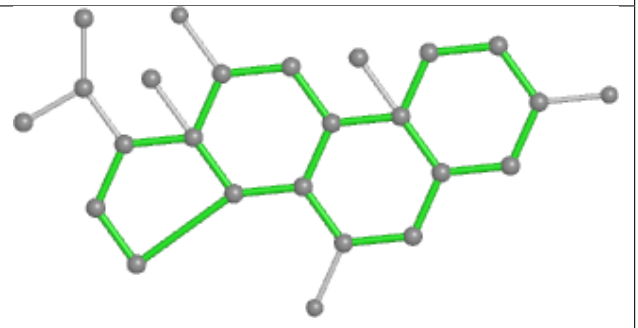
Bond lengths



Bond angles

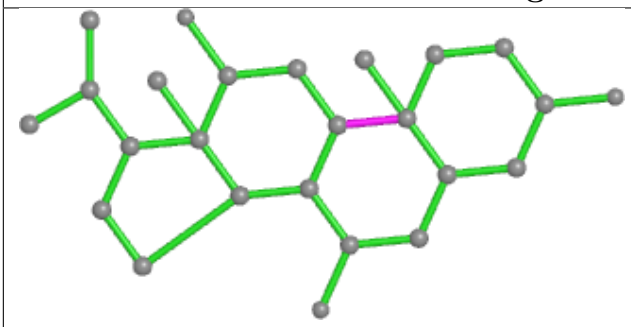


Torsions

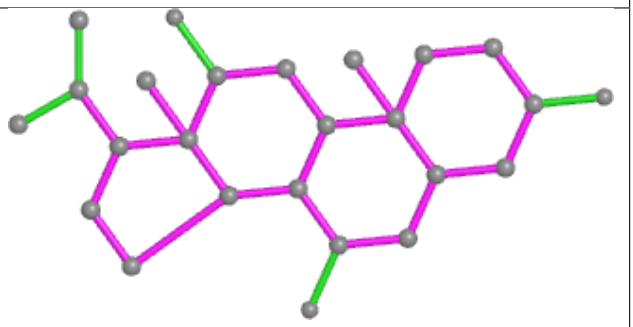


Rings

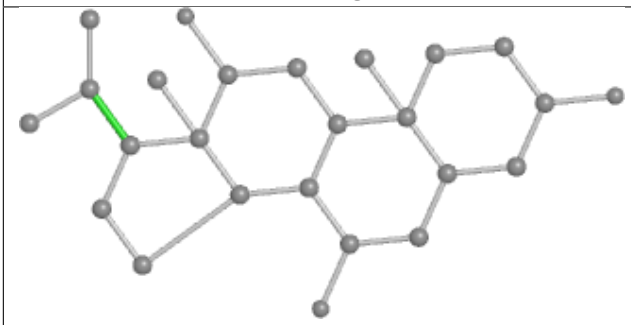
Ligand CPS B 301



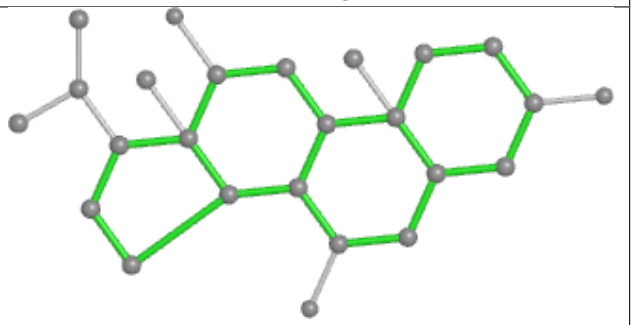
Bond lengths



Bond angles

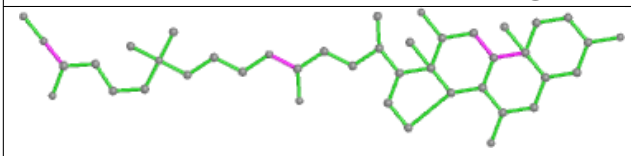


Torsions

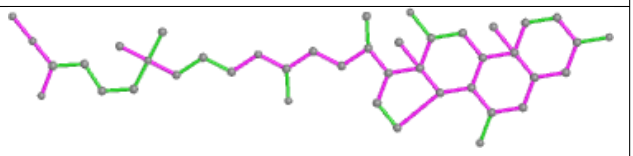


Rings

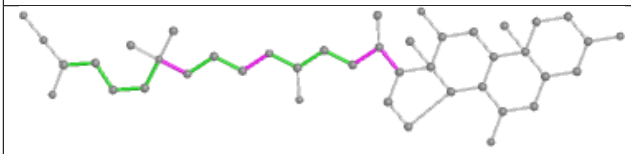
Ligand CPS B 303



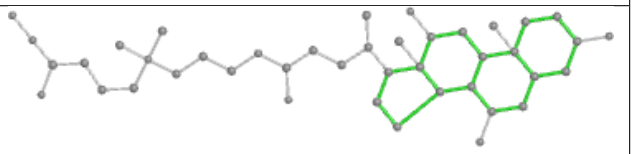
Bond lengths



Bond angles

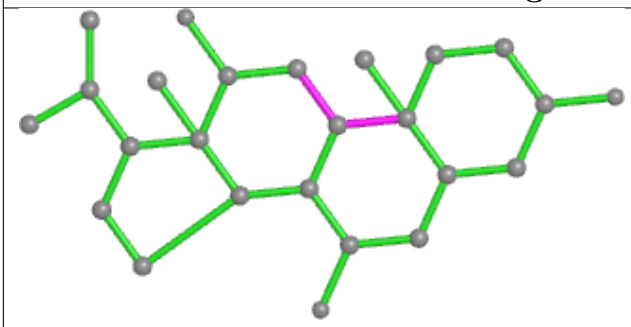


Torsions

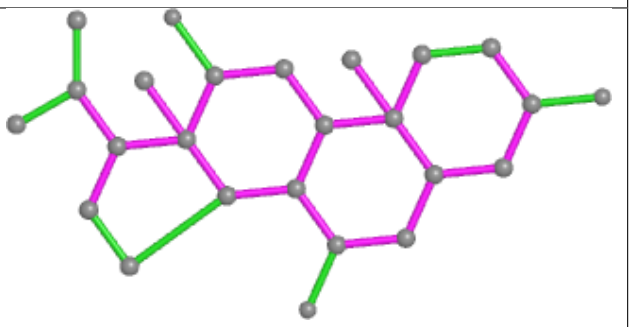


Rings

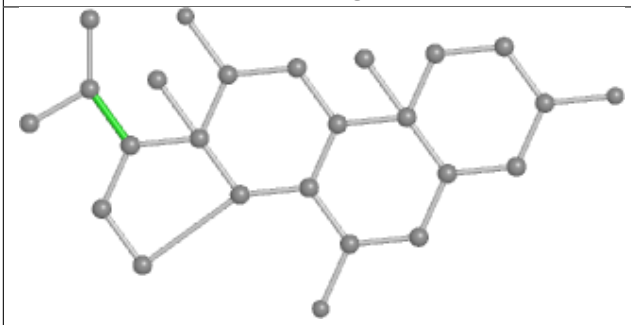
Ligand CPS A 304



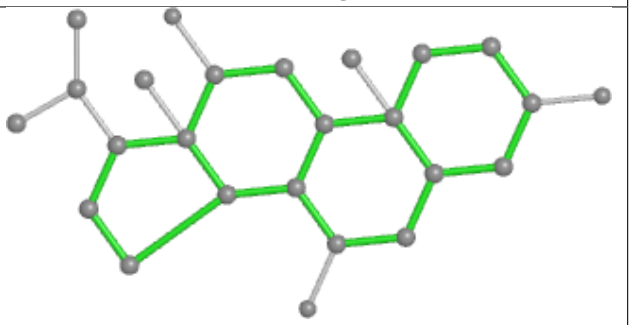
Bond lengths



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

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.