Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:26 AM EDT

PDB ID	:	2E9V
Title	:	Structure of h-CHK1 complexed with A859017
Authors	:	Park, C.
Deposited on	:	2007-01-27
Resolution	:	2.00 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 (1)) were used in the production of this report:

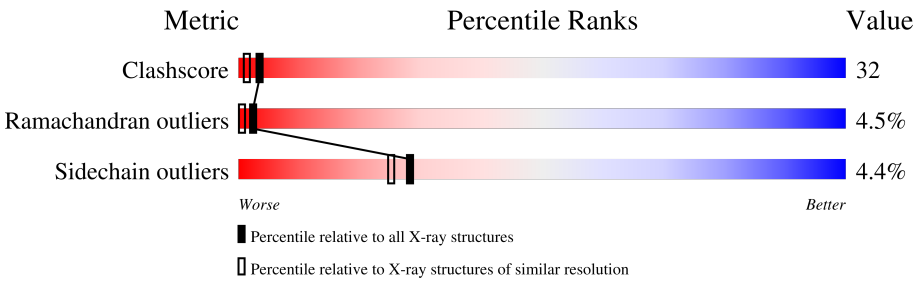
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	268	58% 36% 6%
1	B	268	54% 40% 5% •

2 Entry composition (i)

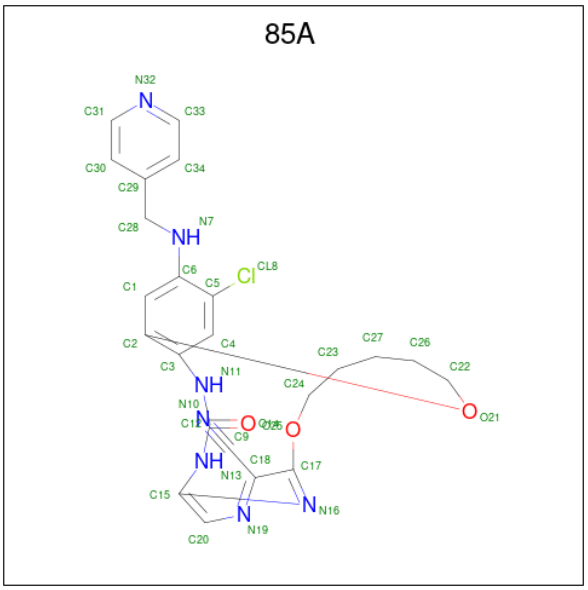
There are 3 unique types of molecules in this entry. The entry contains 4850 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine/threonine-protein kinase Chk1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2176	1393	373	398	12	0	0	0
1	B	268	2176	1393	373	398	12	0	0	0

- Molecule 2 is 18-CHLORO-2-OXO-17-[(PYRIDIN-4-YLMETHYL)AMINO]-2,3,11,12,13,14-HEXAHYDRO-1H,10H-4,8-(AZENO)-9,15,1,3,6-BENZODIOXATRIAZACYCLOHEPTADECINE-7-CARBONITRILE (three-letter code: 85A) (formula: $C_{23}H_{22}ClN_7O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	34	23	1	7	3	0	0
2	B	1	34	23	1	7	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	206	206	206	0	0
			Total	O		
3	B	224	224	224	0	0

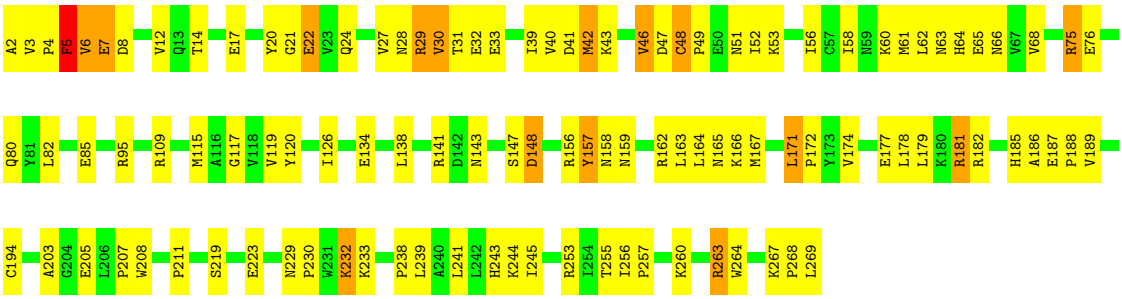
3 Residue-property plots (i)

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.

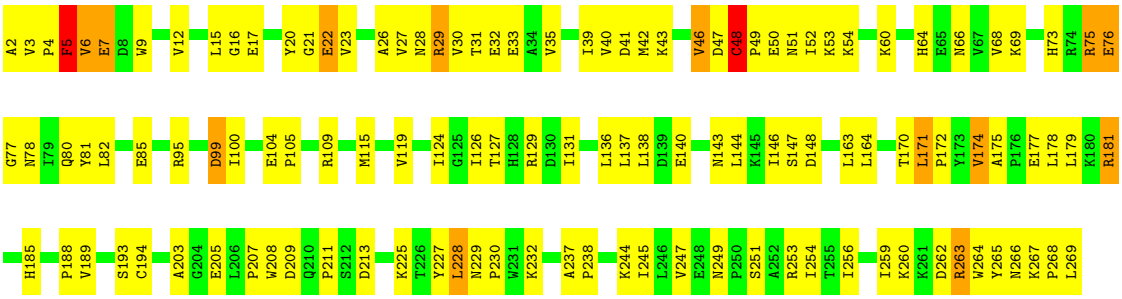
• Molecule 1: Serine/threonine-protein kinase Chk1

Chain A: 58% 36% 6%



• Molecule 1: Serine/threonine-protein kinase Chk1

Chain B: 54% 40% 5% •



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	45.88Å 56.78Å 64.59Å 92.83° 104.39° 113.86°	Depositor
Resolution (Å)	19.77 – 2.00	Depositor
% Data completeness (in resolution range)	72.3 (19.77-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.257 , 0.333	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4850	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

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: 85A

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	0.34	0/2229	0.60	0/3021
1	B	0.33	0/2229	0.61	0/3021
All	All	0.34	0/4458	0.61	0/6042

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 (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	2176	0	2163	149	0
1	B	2176	0	2163	149	0
2	A	34	0	22	1	0
2	B	34	0	22	2	0
3	A	206	0	0	5	0
3	B	224	0	0	15	0
All	All	4850	0	4370	283	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 32.

All (283) 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:263:ARG:HH11	1:A:263:ARG:HB3	1.08	1.11
1:A:263:ARG:HB3	1:A:263:ARG:NH1	1.69	1.08
1:B:6:VAL:HG12	1:B:30:VAL:HB	1.37	1.00
1:A:6:VAL:HG12	1:A:30:VAL:HB	1.44	1.00
1:B:263:ARG:HH11	1:B:263:ARG:HB3	1.41	0.84
1:B:28:ASN:HD22	1:B:30:VAL:H	1.25	0.83
1:B:263:ARG:CZ	1:B:263:ARG:H	1.91	0.83
1:A:6:VAL:HA	1:A:28:ASN:HD21	1.44	0.81
1:A:40:VAL:HG13	1:A:80:GLN:HB3	1.63	0.79
1:B:6:VAL:HG11	1:B:31:THR:OG1	1.82	0.79
1:B:170:THR:HG22	1:B:172:PRO:HD2	1.63	0.78
1:B:52:ILE:HD11	1:B:82:LEU:HD11	1.64	0.77
1:B:75:ARG:HD3	1:B:75:ARG:H	1.49	0.77
1:A:75:ARG:H	1:A:75:ARG:HD3	1.50	0.77
1:A:263:ARG:CZ	1:A:263:ARG:H	1.98	0.77
1:A:14:THR:HA	1:A:24:GLN:NE2	2.00	0.76
1:B:263:ARG:HB3	1:B:263:ARG:NH1	2.01	0.75
1:B:95:ARG:NH1	1:B:138:LEU:HD12	2.02	0.74
1:A:28:ASN:HD22	1:A:30:VAL:H	1.36	0.73
1:A:263:ARG:HG2	1:A:264:TRP:H	1.51	0.73
1:B:6:VAL:HB	1:B:28:ASN:ND2	2.04	0.73
1:A:75:ARG:HB3	1:A:80:GLN:HE22	1.54	0.72
1:B:5:PHE:CG	1:B:30:VAL:HG21	2.24	0.72
1:A:256:ILE:HG22	1:A:260:LYS:NZ	2.06	0.71
1:B:4:PRO:O	1:B:5:PHE:HB2	1.90	0.71
1:B:256:ILE:HG22	1:B:260:LYS:NZ	2.06	0.70
1:A:6:VAL:HB	1:A:28:ASN:ND2	2.07	0.69
1:A:33:GLU:HG2	3:B:2126:HOH:O	1.92	0.69
1:A:109:ARG:NH2	1:A:143:ASN:OD1	2.26	0.69
1:A:263:ARG:NH1	1:B:3:VAL:HB	2.07	0.69
1:A:263:ARG:CZ	1:B:3:VAL:HB	2.22	0.69
1:B:40:VAL:HG13	1:B:80:GLN:HB3	1.73	0.68
1:B:245:ILE:O	1:B:253:ARG:HD2	1.94	0.68
1:A:263:ARG:HG2	1:A:264:TRP:N	2.06	0.68
1:A:6:VAL:HG21	1:A:31:THR:OG1	1.94	0.67
1:B:174:VAL:O	1:B:211:PRO:HG3	1.93	0.67
1:A:177:GLU:HG2	1:A:178:LEU:HD12	1.77	0.66
1:B:181:ARG:HG2	3:B:2103:HOH:O	1.94	0.66
1:A:6:VAL:HG12	1:A:30:VAL:CB	2.24	0.66
1:A:75:ARG:CB	1:A:80:GLN:HE22	2.08	0.66
1:A:21:GLY:HA3	1:A:39:ILE:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CG	1:A:30:VAL:HG21	2.31	0.65
1:B:17:GLU:HA	1:B:22:GLU:HA	1.76	0.65
1:A:165:ASN:HB2	1:A:182:ARG:O	1.95	0.65
1:B:266:ASN:O	1:B:268:PRO:HD3	1.97	0.65
1:A:164:LEU:HD22	1:A:186:ALA:HB2	1.79	0.65
1:B:245:ILE:HB	3:B:2124:HOH:O	1.95	0.65
1:A:6:VAL:CA	1:A:28:ASN:HD21	2.10	0.64
1:B:95:ARG:HD3	3:B:2070:HOH:O	1.96	0.64
1:A:6:VAL:HG11	1:A:31:THR:OG1	1.96	0.64
1:B:42:MET:HB3	1:B:48:CYS:SG	2.37	0.64
1:B:177:GLU:HG2	1:B:178:LEU:HD12	1.80	0.64
1:A:95:ARG:NH1	1:A:138:LEU:HD12	2.12	0.64
1:A:263:ARG:NH1	1:A:263:ARG:CB	2.56	0.63
1:A:58:ILE:HG23	1:A:126:ILE:HD13	1.81	0.63
1:B:244:LYS:NZ	1:B:263:ARG:HH21	1.98	0.62
1:A:48:CYS:HB3	1:A:49:PRO:HD3	1.80	0.62
1:B:21:GLY:O	1:B:22:GLU:HB3	1.99	0.62
1:A:174:VAL:O	1:A:211:PRO:HG3	2.00	0.61
1:B:6:VAL:HA	1:B:28:ASN:HD21	1.65	0.61
1:B:21:GLY:HA3	1:B:39:ILE:O	2.00	0.61
1:B:177:GLU:OE2	1:B:253:ARG:NH2	2.30	0.61
1:B:48:CYS:H	1:B:49:PRO:CD	2.14	0.61
1:B:262:ASP:HA	1:B:263:ARG:NH2	2.16	0.60
1:A:141:ARG:HH22	1:B:126:ILE:CD1	2.14	0.60
1:B:99:ASP:O	1:B:100:ILE:HD13	2.01	0.60
1:B:203:ALA:HB1	1:B:230:PRO:HB2	1.82	0.59
1:A:239:LEU:HG	1:A:243:HIS:HE1	1.67	0.59
1:B:64:HIS:HE1	1:B:66:ASN:HD22	1.48	0.59
1:A:95:ARG:HG3	1:A:138:LEU:HD11	1.85	0.59
1:B:46:VAL:HG13	1:B:47:ASP:N	2.17	0.59
1:A:219:SER:O	1:A:223:GLU:HG3	2.03	0.59
1:B:263:ARG:HG2	1:B:264:TRP:N	2.16	0.59
1:B:203:ALA:CB	1:B:230:PRO:HB2	2.33	0.58
1:B:48:CYS:N	1:B:51:ASN:ND2	2.51	0.58
1:A:177:GLU:OE2	1:A:253:ARG:NH2	2.35	0.58
1:A:268:PRO:HD2	1:B:33:GLU:OE1	2.03	0.58
1:B:119:VAL:HG22	1:B:256:ILE:HG21	1.85	0.58
1:A:267:LYS:HE2	1:A:269:LEU:HD21	1.85	0.58
1:B:48:CYS:H	1:B:49:PRO:HD2	1.67	0.58
1:A:68:VAL:HG13	1:A:85:GLU:HB3	1.84	0.58
1:B:75:ARG:CB	1:B:80:GLN:HE22	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:THR:O	1:B:32:GLU:HB2	2.04	0.57
1:A:244:LYS:HD3	3:B:2026:HOH:O	2.03	0.57
1:B:75:ARG:HD3	1:B:75:ARG:N	2.18	0.57
1:B:5:PHE:CD2	1:B:30:VAL:HG21	2.39	0.57
1:A:40:VAL:CG1	1:A:80:GLN:HB3	2.34	0.57
1:A:141:ARG:NH2	1:B:124:ILE:HD12	2.19	0.57
1:B:54:LYS:HD3	3:B:2053:HOH:O	2.04	0.57
1:A:134:GLU:HB3	3:A:1154:HOH:O	2.05	0.57
1:A:31:THR:O	1:A:32:GLU:HB2	2.05	0.56
1:B:205:GLU:CG	1:B:230:PRO:HB3	2.35	0.56
1:A:238:PRO:HD3	1:A:264:TRP:CD1	2.40	0.56
1:A:241:LEU:HA	1:A:244:LYS:HE3	1.87	0.56
1:A:61:MET:SD	1:A:126:ILE:HD11	2.46	0.56
1:A:239:LEU:HG	1:A:243:HIS:CE1	2.41	0.55
1:A:268:PRO:HD2	1:B:33:GLU:CD	2.26	0.55
1:A:64:HIS:HE1	1:A:66:ASN:HD22	1.54	0.55
1:A:165:ASN:CB	1:A:182:ARG:O	2.54	0.55
1:A:31:THR:CG2	1:A:33:GLU:HG3	2.36	0.55
1:B:256:ILE:HG22	1:B:260:LYS:HZ2	1.71	0.55
1:B:163:LEU:HD21	1:B:185:HIS:CE1	2.42	0.55
1:B:256:ILE:HG22	1:B:260:LYS:HZ1	1.72	0.55
1:A:12:VAL:HG21	1:A:27:VAL:HG23	1.87	0.54
1:A:232:LYS:O	1:A:232:LYS:HG2	2.07	0.54
1:B:75:ARG:HB3	1:B:80:GLN:HE22	1.71	0.54
1:B:6:VAL:HB	1:B:28:ASN:CG	2.28	0.54
1:B:263:ARG:HG2	1:B:264:TRP:H	1.72	0.54
1:A:48:CYS:N	1:A:51:ASN:ND2	2.56	0.54
1:A:141:ARG:HH12	1:B:126:ILE:HG13	1.73	0.53
1:B:6:VAL:O	1:B:7:GLU:HB2	2.09	0.53
1:B:17:GLU:HB3	1:B:22:GLU:HB2	1.90	0.53
1:B:28:ASN:HD22	1:B:30:VAL:N	2.01	0.53
1:A:48:CYS:N	1:A:51:ASN:HD22	2.06	0.53
1:B:68:VAL:HG21	1:B:147:SER:HB3	1.89	0.53
1:B:119:VAL:CG2	1:B:256:ILE:HG21	2.39	0.53
1:B:75:ARG:HB3	1:B:80:GLN:NE2	2.24	0.53
1:A:255:THR:HB	1:A:257:PRO:HD2	1.91	0.52
1:B:68:VAL:HG13	1:B:85:GLU:HB3	1.90	0.52
1:A:5:PHE:CB	1:A:30:VAL:HG21	2.39	0.52
1:A:17:GLU:HB3	1:A:22:GLU:HB3	1.91	0.52
1:A:157:TYR:C	1:A:159:ASN:N	2.61	0.52
1:B:9:TRP:CZ3	1:B:35:VAL:HG22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:MET:HA	3:A:1017:HOH:O	2.09	0.52
1:A:42:MET:HB3	1:A:48:CYS:SG	2.50	0.52
1:B:73:HIS:CE1	1:B:75:ARG:HD2	2.45	0.51
1:A:141:ARG:HG2	1:B:124:ILE:HB	1.92	0.51
1:A:5:PHE:CD2	1:A:30:VAL:HG21	2.44	0.51
1:A:42:MET:CB	1:A:48:CYS:SG	2.98	0.51
1:B:189:VAL:HG11	3:B:2084:HOH:O	2.11	0.51
1:A:31:THR:HG21	1:A:33:GLU:CD	2.31	0.51
1:A:119:VAL:CG2	1:A:256:ILE:HG21	2.41	0.51
1:A:256:ILE:HG22	1:A:260:LYS:HZ1	1.75	0.51
1:B:41:ASP:OD1	1:B:43:LYS:N	2.43	0.51
1:A:4:PRO:O	1:A:5:PHE:HB2	2.11	0.50
1:A:205:GLU:HG3	1:A:230:PRO:HB3	1.94	0.50
1:A:245:ILE:O	1:A:253:ARG:HD2	2.09	0.50
1:B:68:VAL:HG11	2:B:2001:85A:H20	1.93	0.50
1:A:68:VAL:HG21	1:A:147:SER:HB3	1.94	0.50
1:A:6:VAL:O	1:A:7:GLU:HB2	2.11	0.50
1:A:7:GLU:HG2	1:A:7:GLU:O	2.11	0.50
1:A:205:GLU:CG	1:A:230:PRO:HB3	2.41	0.49
1:B:9:TRP:HB3	1:B:26:ALA:HB1	1.94	0.49
1:B:207:PRO:HB2	1:B:208:TRP:CE3	2.47	0.49
1:A:256:ILE:HG22	1:A:260:LYS:HZ2	1.77	0.49
1:A:21:GLY:O	1:A:22:GLU:HB3	2.10	0.49
1:A:46:VAL:HG13	1:A:47:ASP:N	2.28	0.49
1:A:177:GLU:CD	1:A:253:ARG:HH22	2.16	0.49
1:B:4:PRO:O	1:B:5:PHE:CB	2.61	0.49
1:B:48:CYS:SG	1:B:49:PRO:HD3	2.53	0.49
1:B:52:ILE:HD11	1:B:82:LEU:CD1	2.39	0.49
1:A:31:THR:HG22	1:A:33:GLU:HG3	1.95	0.48
1:A:157:TYR:C	1:A:159:ASN:H	2.15	0.48
1:B:225:LYS:O	1:B:228:LEU:HB2	2.13	0.48
1:B:5:PHE:CB	1:B:30:VAL:HG21	2.44	0.48
1:A:52:ILE:HD11	1:A:82:LEU:HD21	1.96	0.48
1:A:56:ILE:O	1:A:60:LYS:HG3	2.12	0.48
1:B:6:VAL:CB	1:B:28:ASN:HD21	2.27	0.48
1:B:52:ILE:HG23	1:B:53:LYS:N	2.28	0.48
1:B:205:GLU:CD	1:B:230:PRO:HB3	2.34	0.48
1:A:6:VAL:CB	1:A:31:THR:OG1	2.62	0.48
1:A:52:ILE:O	1:A:56:ILE:HG13	2.13	0.48
1:A:269:LEU:O	1:B:69:LYS:NZ	2.47	0.48
1:B:205:GLU:OE2	1:B:230:PRO:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:HH22	1:B:126:ILE:HD11	1.79	0.47
1:B:104:GLU:N	1:B:105:PRO:CD	2.77	0.47
1:B:178:LEU:C	1:B:179:LEU:HD12	2.35	0.47
1:A:14:THR:HA	1:A:24:GLN:HE22	1.80	0.47
1:B:115:MET:O	1:B:119:VAL:HG23	2.14	0.47
1:A:162:ARG:HG2	1:A:163:LEU:N	2.30	0.47
1:B:75:ARG:O	1:B:76:GLU:C	2.53	0.47
1:A:75:ARG:HD3	1:A:75:ARG:N	2.26	0.47
1:A:7:GLU:N	1:A:28:ASN:OD1	2.48	0.47
1:A:141:ARG:NH2	1:B:126:ILE:HD11	2.30	0.47
1:B:48:CYS:N	1:B:49:PRO:CD	2.74	0.47
1:B:127:THR:HG23	1:B:129:ARG:HG3	1.96	0.47
1:B:6:VAL:CA	1:B:28:ASN:HD21	2.27	0.46
1:B:48:CYS:SG	1:B:49:PRO:N	2.87	0.46
1:B:5:PHE:CD2	1:B:30:VAL:CG2	2.98	0.46
1:A:5:PHE:CD2	1:A:30:VAL:CG2	2.99	0.46
1:A:6:VAL:O	1:A:6:VAL:CG2	2.63	0.46
1:A:17:GLU:HB3	1:A:22:GLU:CB	2.45	0.46
1:B:68:VAL:HG21	1:B:147:SER:CB	2.45	0.46
1:A:5:PHE:O	1:A:30:VAL:CG2	2.64	0.46
1:B:164:LEU:HB3	3:B:2031:HOH:O	2.16	0.46
1:B:227:TYR:CE1	1:B:228:LEU:HD13	2.49	0.46
1:A:207:PRO:HB2	1:A:208:TRP:CE3	2.50	0.46
1:A:6:VAL:CB	1:A:28:ASN:HD21	2.29	0.46
1:B:136:LEU:CD2	1:B:146:ILE:HG12	2.46	0.46
1:A:115:MET:HE3	1:A:194:CYS:HB3	1.97	0.46
1:A:119:VAL:HG23	1:A:256:ILE:HG21	1.98	0.46
1:B:5:PHE:O	1:B:30:VAL:CG2	2.64	0.46
1:A:51:ASN:HB3	3:A:1068:HOH:O	2.17	0.45
1:B:2:ALA:O	1:B:3:VAL:HG22	2.16	0.45
1:A:187:GLU:HB2	1:A:188:PRO:HD3	1.99	0.45
1:A:82:LEU:N	1:A:82:LEU:HD12	2.32	0.45
1:A:30:VAL:O	1:A:32:GLU:HG3	2.17	0.45
1:B:49:PRO:HB2	1:B:50:GLU:OE2	2.16	0.45
1:B:12:VAL:HG21	1:B:27:VAL:HG23	1.98	0.45
1:B:28:ASN:C	1:B:30:VAL:H	2.21	0.45
1:A:134:GLU:OE1	1:A:134:GLU:N	2.49	0.44
1:A:178:LEU:HD11	1:A:189:VAL:CG2	2.47	0.44
1:A:75:ARG:HB3	1:A:80:GLN:NE2	2.30	0.44
1:B:171:LEU:HB2	1:B:172:PRO:HD3	2.00	0.44
1:A:6:VAL:CG1	1:A:31:THR:OG1	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD12	1:B:23:VAL:HG12	2.00	0.44
1:A:163:LEU:HD21	1:A:185:HIS:CD2	2.51	0.44
1:B:164:LEU:HD23	3:B:2031:HOH:O	2.17	0.44
1:A:156:ARG:NH2	1:A:187:GLU:CD	2.71	0.44
1:A:174:VAL:HG11	1:A:179:LEU:HD11	1.99	0.44
1:B:174:VAL:HG13	1:B:175:ALA:O	2.18	0.44
1:A:41:ASP:HB3	3:A:1142:HOH:O	2.17	0.44
1:A:256:ILE:N	1:A:257:PRO:CD	2.81	0.44
1:B:48:CYS:N	1:B:51:ASN:HD22	2.15	0.44
1:B:174:VAL:HG22	1:B:178:LEU:HD22	2.00	0.44
1:B:52:ILE:HG12	1:B:80:GLN:HG2	1.99	0.43
1:B:2:ALA:C	1:B:3:VAL:CG2	2.86	0.43
1:B:28:ASN:ND2	1:B:30:VAL:H	2.04	0.43
1:B:42:MET:HG2	3:B:2117:HOH:O	2.18	0.43
1:A:14:THR:CA	1:A:24:GLN:HE22	2.31	0.43
1:B:69:LYS:HG3	3:B:2085:HOH:O	2.18	0.43
1:B:237:ALA:HB3	1:B:238:PRO:CD	2.48	0.43
1:A:117:GLY:O	1:A:120:TYR:HB3	2.19	0.43
1:B:28:ASN:O	1:B:30:VAL:N	2.51	0.43
1:B:249:ASN:OD1	1:B:251:SER:HB2	2.19	0.43
1:A:2:ALA:O	1:A:3:VAL:HG22	2.19	0.43
1:A:6:VAL:CB	1:A:28:ASN:ND2	2.79	0.43
1:A:58:ILE:O	1:A:62:LEU:HG	2.18	0.43
1:A:75:ARG:H	1:A:75:ARG:CD	2.24	0.43
1:A:5:PHE:HB3	1:A:30:VAL:HG11	2.01	0.42
1:B:267:LYS:HG2	1:B:269:LEU:HD21	2.01	0.42
1:A:165:ASN:OD1	1:A:166:LYS:N	2.52	0.42
1:A:167:MET:HG2	1:A:178:LEU:O	2.20	0.42
1:A:263:ARG:CG	1:A:264:TRP:N	2.78	0.42
1:A:6:VAL:CG2	1:A:31:THR:OG1	2.63	0.42
1:A:53:LYS:HA	1:A:53:LYS:HD3	1.79	0.42
1:A:158:ASN:O	1:A:159:ASN:HB3	2.19	0.42
1:A:229:ASN:ND2	1:A:233:LYS:HG3	2.34	0.42
1:B:260:LYS:HA	1:B:265:TYR:CD2	2.55	0.42
1:B:6:VAL:O	1:B:6:VAL:CG2	2.67	0.42
1:B:245:ILE:HA	1:B:254:ILE:HG22	2.02	0.42
1:B:16:GLY:HA3	2:B:2001:85A:H262	2.01	0.42
1:B:48:CYS:SG	1:B:49:PRO:CD	3.08	0.42
1:A:31:THR:HG21	1:A:33:GLU:HG3	2.02	0.42
1:B:109:ARG:HD3	3:B:2095:HOH:O	2.18	0.42
1:B:229:ASN:HD22	1:B:229:ASN:HA	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:CD	1:A:269:LEU:HD21	2.50	0.42
1:B:77:GLY:O	1:B:78:ASN:ND2	2.53	0.42
1:B:164:LEU:N	1:B:164:LEU:CD1	2.83	0.42
1:A:178:LEU:HD11	1:A:189:VAL:HG21	2.02	0.41
1:A:141:ARG:HH12	1:B:126:ILE:CG1	2.34	0.41
1:B:6:VAL:CB	1:B:28:ASN:ND2	2.76	0.41
1:B:46:VAL:CG1	1:B:47:ASP:N	2.81	0.41
1:A:41:ASP:C	1:A:43:LYS:H	2.24	0.41
1:A:148:ASP:HA	2:A:1001:85A:N10	2.35	0.41
1:B:137:LEU:O	1:B:144:LEU:HA	2.20	0.41
1:B:247:VAL:O	1:B:253:ARG:HD3	2.20	0.41
1:A:6:VAL:HG12	1:A:30:VAL:CG1	2.50	0.41
1:A:6:VAL:HB	1:A:28:ASN:HD21	1.83	0.41
1:B:175:ALA:HB1	1:B:177:GLU:OE1	2.21	0.41
1:A:171:LEU:CB	1:A:172:PRO:HD3	2.51	0.41
1:A:243:HIS:HD2	3:A:1002:HOH:O	2.02	0.41
1:B:263:ARG:H	1:B:263:ARG:NH1	2.17	0.41
1:A:2:ALA:C	1:A:3:VAL:CG2	2.89	0.41
1:B:28:ASN:C	1:B:30:VAL:N	2.75	0.41
1:B:39:ILE:HD12	1:B:81:TYR:CE2	2.55	0.41
1:B:64:HIS:HE1	1:B:66:ASN:ND2	2.15	0.41
1:B:109:ARG:NH2	1:B:143:ASN:OD1	2.53	0.41
1:B:209:ASP:HB3	3:B:2109:HOH:O	2.19	0.41
1:A:177:GLU:O	1:A:181:ARG:HB2	2.21	0.41
1:A:263:ARG:HD3	1:B:3:VAL:HG11	2.03	0.41
1:B:75:ARG:CB	1:B:80:GLN:NE2	2.83	0.41
1:B:259:ILE:O	1:B:262:ASP:HB3	2.21	0.41
1:A:141:ARG:HH21	1:B:124:ILE:HD12	1.84	0.40
1:A:255:THR:CB	1:A:257:PRO:HD2	2.51	0.40
1:B:27:VAL:HB	3:B:2157:HOH:O	2.21	0.40
1:A:30:VAL:C	1:A:32:GLU:N	2.73	0.40
1:A:65:GLU:OE1	1:B:60:LYS:NZ	2.54	0.40
1:A:203:ALA:CB	1:A:230:PRO:HB2	2.51	0.40
1:B:115:MET:CE	1:B:194:CYS:SG	3.10	0.40
1:B:188:PRO:HB2	3:B:2066:HOH:O	2.20	0.40
1:A:75:ARG:N	1:A:75:ARG:CD	2.85	0.40
1:B:131:ILE:HB	1:B:193:SER:OG	2.21	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	266/268 (99%)	232 (87%)	20 (8%)	14 (5%)	2 0
1	B	266/268 (99%)	231 (87%)	25 (9%)	10 (4%)	3 1
All	All	532/536 (99%)	463 (87%)	45 (8%)	24 (4%)	2 0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	7	GLU
1	A	20	TYR
1	A	46	VAL
1	B	5	PHE
1	B	7	GLU
1	B	46	VAL
1	B	76	GLU
1	A	48	CYS
1	B	48	CYS
1	A	42	MET
1	A	76	GLU
1	A	148	ASP
1	B	22	GLU
1	B	29	ARG
1	A	22	GLU
1	A	157	TYR
1	B	20	TYR
1	B	148	ASP
1	A	29	ARG
1	A	63	ASN
1	A	30	VAL
1	A	171	LEU
1	B	171	LEU

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	237/237 (100%)	229 (97%)	8 (3%)	37	36
1	B	237/237 (100%)	224 (94%)	13 (6%)	21	17
All	All	474/474 (100%)	453 (96%)	21 (4%)	28	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	6	VAL
1	A	8	ASP
1	A	29	ARG
1	A	75	ARG
1	A	181	ARG
1	A	232	LYS
1	A	263	ARG
1	B	5	PHE
1	B	6	VAL
1	B	29	ARG
1	B	48	CYS
1	B	75	ARG
1	B	99	ASP
1	B	140	GLU
1	B	174	VAL
1	B	181	ARG
1	B	213	ASP
1	B	228	LEU
1	B	232	LYS
1	B	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN

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Mol	Chain	Res	Type
1	A	28	ASN
1	A	51	ASN
1	A	66	ASN
1	A	78	ASN
1	A	80	GLN
1	A	113	GLN
1	A	135	ASN
1	A	158	ASN
1	A	185	HIS
1	A	229	ASN
1	B	28	ASN
1	B	51	ASN
1	B	66	ASN
1	B	73	HIS
1	B	78	ASN
1	B	80	GLN
1	B	113	GLN
1	B	135	ASN
1	B	229	ASN

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)

2 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	85A	B	2001	-	37,37,37	2.90	14 (37%)	49,49,49	3.56	14 (28%)
2	85A	A	1001	-	37,37,37	3.11	14 (37%)	49,49,49	3.72	13 (26%)

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	85A	B	2001	-	-	9/23/25/25	0/3/4/4
2	85A	A	1001	-	-	9/23/25/25	0/3/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	85A	C17-N16	7.96	1.43	1.32
2	B	2001	85A	C17-N16	7.45	1.42	1.32
2	A	1001	85A	C18-C17	6.56	1.48	1.43
2	B	2001	85A	C1-C2	6.50	1.49	1.38
2	A	1001	85A	C1-C2	6.44	1.49	1.38
2	A	1001	85A	O25-C17	6.20	1.44	1.34
2	A	1001	85A	C18-N19	6.07	1.39	1.34
2	B	2001	85A	C18-C17	5.60	1.47	1.43
2	B	2001	85A	C18-N19	5.36	1.39	1.34
2	A	1001	85A	C4-C3	5.31	1.47	1.39
2	B	2001	85A	C4-C3	5.21	1.47	1.39
2	A	1001	85A	C15-N16	5.10	1.44	1.34
2	B	2001	85A	O25-C17	4.75	1.42	1.34
2	B	2001	85A	C15-N16	4.55	1.43	1.34
2	B	2001	85A	C3-C2	3.87	1.48	1.40
2	A	1001	85A	C3-C2	3.81	1.48	1.40
2	B	2001	85A	C1-C6	3.46	1.45	1.39
2	A	1001	85A	C1-C6	3.38	1.44	1.39
2	A	1001	85A	O21-C2	2.59	1.42	1.37
2	B	2001	85A	C20-N19	2.48	1.39	1.34
2	A	1001	85A	C20-N19	2.48	1.39	1.34
2	A	1001	85A	C12-N11	2.45	1.42	1.37
2	B	2001	85A	C12-N11	2.44	1.42	1.37
2	B	2001	85A	C4-C5	2.44	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	85A	C4-C5	2.38	1.42	1.38
2	B	2001	85A	C6-C5	2.35	1.45	1.39
2	A	1001	85A	C6-C5	2.33	1.45	1.39
2	B	2001	85A	O21-C2	2.20	1.41	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	85A	O25-C17-C18	19.23	127.00	116.13
2	B	2001	85A	O25-C17-C18	17.86	126.22	116.13
2	A	1001	85A	C18-C17-N16	-9.72	118.64	121.86
2	B	2001	85A	C18-C17-N16	-7.37	119.42	121.86
2	B	2001	85A	C17-C18-N19	-6.35	119.69	122.23
2	B	2001	85A	C20-C15-N16	-5.93	118.70	121.94
2	A	1001	85A	C27-C26-C22	-5.31	90.40	113.47
2	A	1001	85A	C20-C15-N16	-5.28	119.05	121.94
2	B	2001	85A	C27-C26-C22	-5.05	91.52	113.47
2	A	1001	85A	C17-C18-N19	-4.91	120.27	122.23
2	B	2001	85A	C27-C23-C24	-4.62	93.37	113.47
2	A	1001	85A	C27-C23-C24	-4.60	93.47	113.47
2	A	1001	85A	C20-N19-C18	4.44	120.82	116.97
2	B	2001	85A	C20-N19-C18	4.41	120.79	116.97
2	A	1001	85A	O25-C17-N16	-4.24	114.36	120.02
2	B	2001	85A	O25-C17-N16	-4.24	114.36	120.02
2	B	2001	85A	C9-C18-N19	3.75	122.31	115.23
2	A	1001	85A	O14-C12-N13	-3.49	117.44	123.64
2	A	1001	85A	C15-N13-C12	3.43	136.31	129.91
2	B	2001	85A	O14-C12-N13	-3.42	117.57	123.64
2	B	2001	85A	C15-N13-C12	3.39	136.23	129.91
2	B	2001	85A	C17-C18-C9	-3.30	118.00	120.06
2	B	2001	85A	N13-C12-N11	3.22	118.68	112.44
2	A	1001	85A	N13-C12-N11	2.99	118.22	112.44
2	A	1001	85A	C9-C18-N19	2.99	120.87	115.23
2	B	2001	85A	N13-C15-N16	2.60	119.63	113.33
2	A	1001	85A	N13-C15-N16	2.55	119.51	113.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	85A	C5-C6-N7-C28
2	A	1001	85A	N16-C17-O25-C24

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Mol	Chain	Res	Type	Atoms
2	A	1001	85A	C18-C17-O25-C24
2	B	2001	85A	C5-C6-N7-C28
2	B	2001	85A	N16-C17-O25-C24
2	B	2001	85A	C18-C17-O25-C24
2	B	2001	85A	C1-C6-N7-C28
2	A	1001	85A	C1-C6-N7-C28
2	A	1001	85A	C22-C26-C27-C23
2	B	2001	85A	C24-C23-C27-C26
2	A	1001	85A	C24-C23-C27-C26
2	B	2001	85A	C22-C26-C27-C23
2	B	2001	85A	C26-C22-O21-C2
2	A	1001	85A	C26-C22-O21-C2
2	A	1001	85A	C3-C2-O21-C22
2	A	1001	85A	C1-C2-O21-C22
2	B	2001	85A	C1-C2-O21-C22
2	B	2001	85A	C3-C2-O21-C22

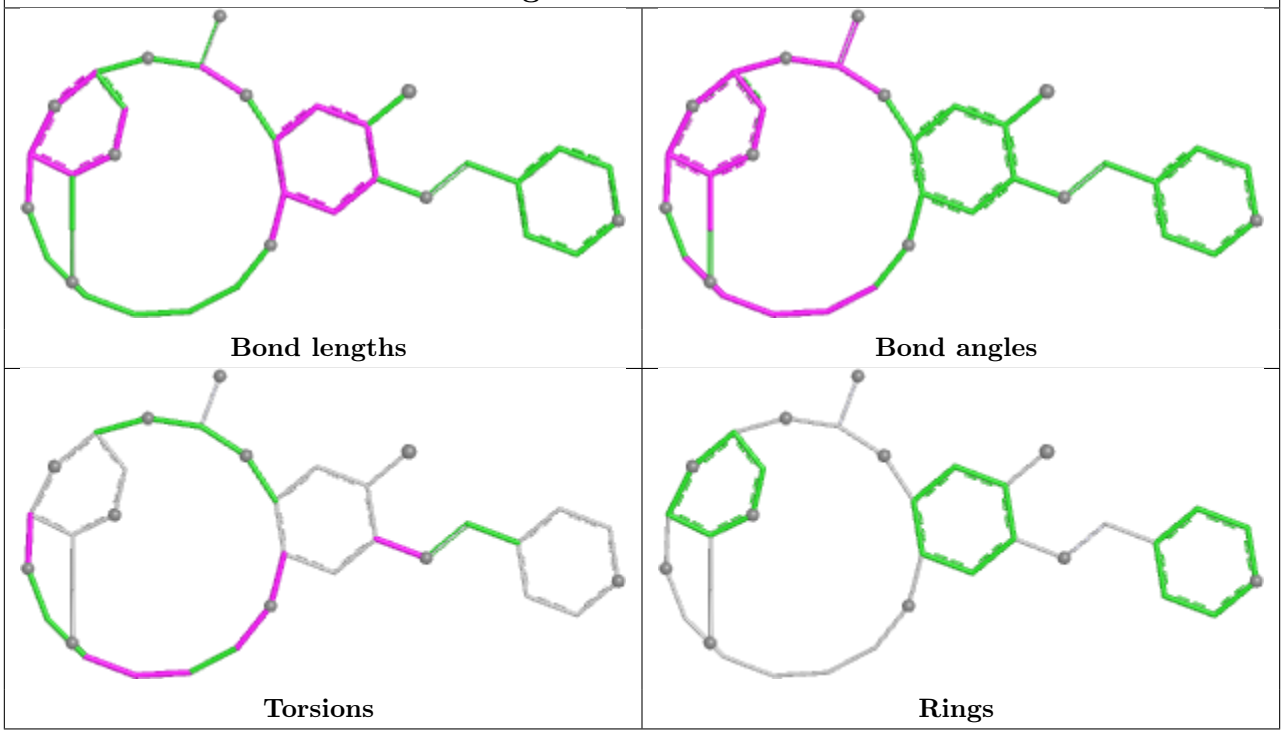
There are no ring outliers.

2 monomers are involved in 3 short contacts:

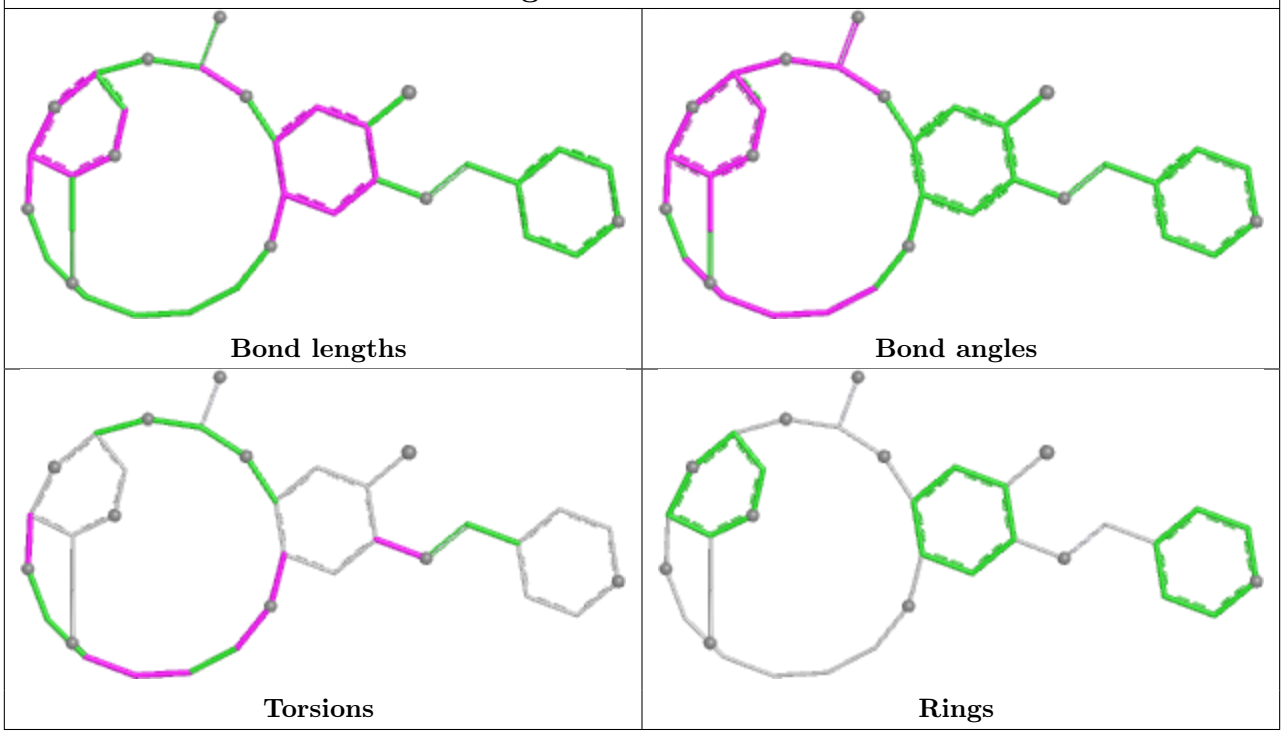
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	85A	2	0
2	A	1001	85A	1	0

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 85A B 2001



Ligand 85A A 1001



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.