Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 01:33 PM EDT

PDB ID	:	4N99
Title	:	E. coli sliding clamp in complex with 6-chloro-2,3,4,9-tetrahydro-1H-carbazole-7-carboxylic acid
Authors	:	Yin, Z.; Oakley, A.J.
Deposited on	:	2013-10-19
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

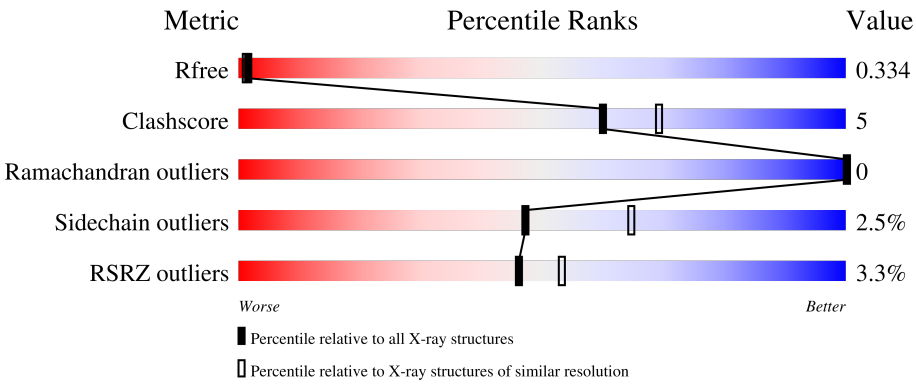
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	366	2% 82% 15%
1	B	366	4% 90% 9%

2 Entry composition (i)

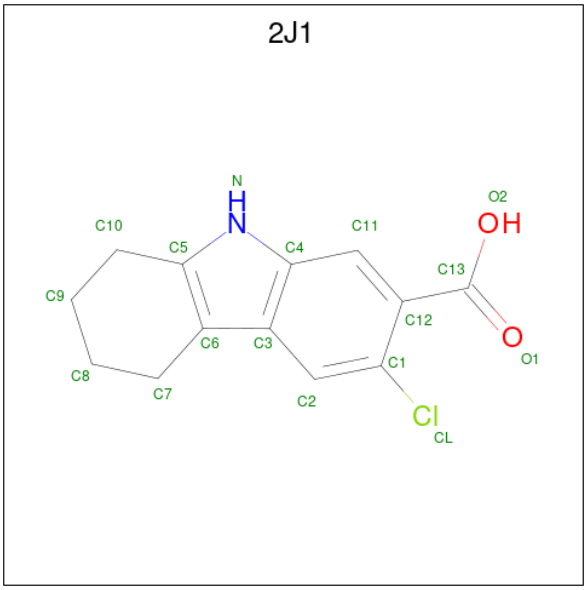
There are 6 unique types of molecules in this entry. The entry contains 6068 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA polymerase III subunit beta.

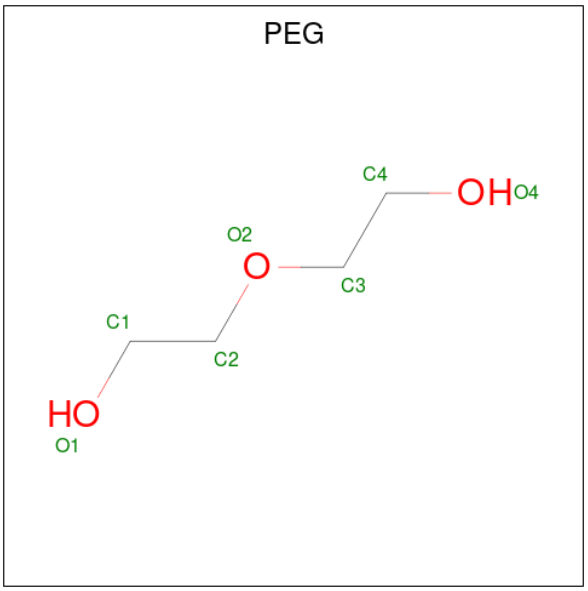
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2732	1725	468	519	20	0	1	0
1	B	365	2818	1771	489	538	20	0	2	0

- Molecule 2 is 6-chloro-2,3,4,9-tetrahydro-1H-carbazole-7-carboxylic acid (three-letter code: 2J1) (formula: $C_{13}H_{12}ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	17	13	1	1	2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4	3		0	0

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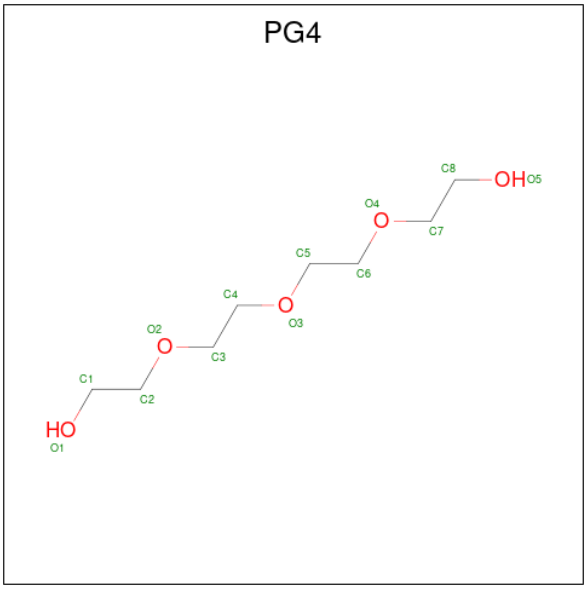
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	13	8	5	0	0
			Total	C	O		
4	B	1	13	8	5	0	0
			Total	C	O		
4	B	1	13	8	5	0	0
			Total	C	O		
4	B	1	13	8	5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	4	4	4	0	0
			Total	Ca		
5	B	1	1	1	0	0

- Molecule 6 is water.

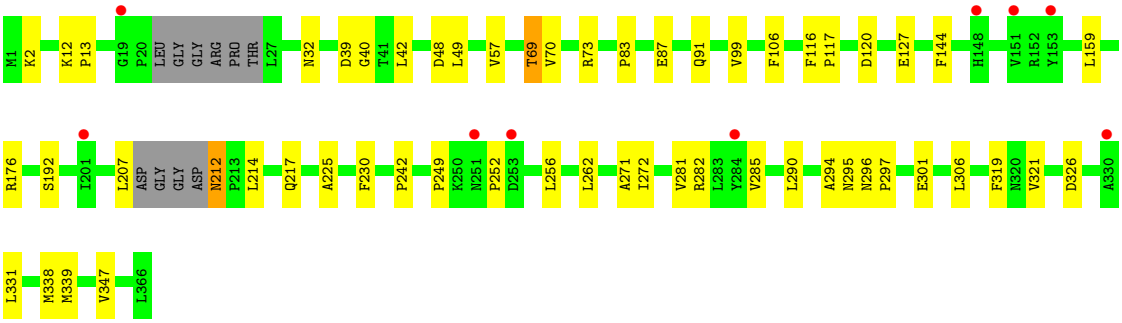
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	120	120	120	0	0
			Total	O		
6	B	113	113	113	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

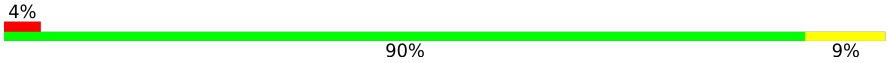
• Molecule 1: DNA polymerase III subunit beta

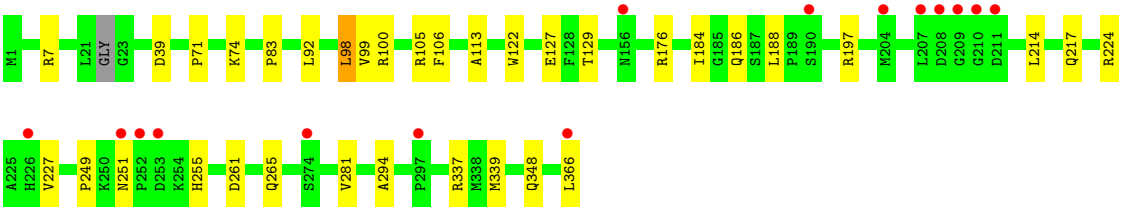
Chain A:



• Molecule 1: DNA polymerase III subunit beta

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.01Å 65.13Å 73.24Å 72.95° 85.06° 85.24°	Depositor
Resolution (Å)	40.95 – 2.30 40.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (40.95-2.30) 92.9 (40.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.261 , 0.338 0.258 , 0.334	Depositor DCC
R_{free} test set	1495 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6068	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2J1, PEG, PG4, CA

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	0.27	0/2781	0.49	0/3768
1	B	0.27	0/2871	0.47	0/3887
All	All	0.27	0/5652	0.48	0/7655

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	2732	0	2719	29	0
1	B	2818	0	2821	22	0
2	A	17	0	11	1	0
3	A	63	0	90	0	0
3	B	70	0	100	4	0
4	A	52	0	72	2	0
4	B	78	0	108	9	0
5	A	4	0	0	0	0
5	B	1	0	0	0	0
6	A	120	0	0	0	0
6	B	113	0	0	0	0
All	All	6068	0	5921	54	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 5.

All (54) 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:32:ASN:HB3	1:A:69:THR:HG22	1.71	0.71
1:A:242:PRO:HB3	2:A:401:2J1:H7	1.75	0.67
1:B:105:ARG:HE	4:B:412:PG4:H22	1.60	0.67
1:A:256:LEU:HB3	1:A:338[B]:MET:HG3	1.80	0.63
1:A:252:PRO:HB2	1:A:339:MET:HB3	1.82	0.61
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.83	0.60
1:A:12:LYS:HB3	1:A:13:PRO:HD3	1.83	0.59
1:B:255:HIS:CD2	1:B:337:ARG:HD2	2.38	0.58
1:B:249:PRO:HD2	1:B:348:GLN:HE21	1.69	0.58
1:A:281:VAL:HG12	1:A:294:ALA:HB2	1.85	0.57
1:B:255:HIS:HD2	1:B:337:ARG:HD2	1.70	0.57
1:B:7:ARG:HH22	4:B:404:PG4:H51	1.69	0.57
3:B:409:PEG:H32	3:B:414:PEG:H31	1.90	0.54
1:A:2:LYS:HG3	1:A:91:GLN:HB3	1.90	0.52
1:B:127:GLU:HG2	1:B:217:GLN:HG2	1.92	0.52
1:B:281:VAL:HG12	1:B:294:ALA:HB2	1.92	0.52
1:B:197:ARG:H	3:B:408:PEG:H31	1.75	0.51
1:B:98:LEU:HD21	1:B:100:ARG:HE	1.75	0.50
1:B:83:PRO:HG3	4:B:401:PG4:C1	2.42	0.50
1:A:99:VAL:HB	1:A:106:PHE:HB2	1.94	0.50
1:A:295:ASN:HB3	1:A:301:GLU:HG2	1.94	0.49
1:A:262:LEU:HD23	4:B:401:PG4:H31	1.94	0.49
1:B:122:TRP:HZ2	1:B:224:ARG:HB2	1.77	0.48
1:A:249:PRO:HB2	1:A:252:PRO:HG3	1.96	0.48
1:A:159:LEU:HD11	1:A:192:SER:HB3	1.96	0.48
1:A:83:PRO:HG3	4:A:410:PG4:O2	2.15	0.47
1:A:127:GLU:HG2	1:A:217:GLN:HG2	1.97	0.47
1:A:271:ALA:HB2	1:A:321:VAL:HG11	1.97	0.46
1:B:129:THR:H	1:B:186:GLN:HE22	1.63	0.46
1:B:71:PRO:HB2	1:B:74:LYS:HB2	1.98	0.45
3:B:410:PEG:H22	3:B:416:PEG:H11	1.98	0.45
1:B:184:ILE:HD11	1:B:188:LEU:HD11	1.99	0.45
1:B:261:ASP:O	1:B:265:GLN:HG2	2.17	0.45
1:A:116:PHE:HA	1:A:117:PRO:HD3	1.88	0.44
1:A:272:ILE:HD11	4:A:404:PG4:H12	1.99	0.44
4:B:401:PG4:H11	3:B:415:PEG:H11	1.99	0.44
1:A:42:LEU:HB3	1:A:57:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:CD2	1:A:326:ASP:HB3	2.53	0.44
1:B:339:MET:HB2	1:B:348:GLN:HB3	2.00	0.43
1:A:285:VAL:HG12	1:A:290:LEU:HD13	2.01	0.43
1:B:92:LEU:HD21	4:B:411:PG4:H62	1.99	0.43
1:A:319:PHE:HZ	1:A:347:VAL:HG21	1.83	0.43
1:A:48:ASP:O	1:A:49:LEU:HB2	2.19	0.42
1:B:113:ALA:H	4:B:411:PG4:H32	1.84	0.42
1:B:83:PRO:HG3	4:B:401:PG4:H12	2.02	0.42
1:A:212:ASN:HD22	1:A:212:ASN:HA	1.70	0.41
1:A:296:ASN:HB2	1:A:297:PRO:CD	2.51	0.41
1:A:296:ASN:HB2	1:A:297:PRO:HD2	2.02	0.41
1:B:105:ARG:CZ	4:B:412:PG4:H61	2.50	0.41
1:B:99:VAL:HB	1:B:106:PHE:HB2	2.03	0.41
1:A:13:PRO:HA	1:A:230:PHE:HE1	1.86	0.41
1:A:39:ASP:HB3	1:A:40:GLY:H	1.74	0.40
1:A:262:LEU:HB3	1:A:306:LEU:HD21	2.04	0.40
1:B:214:LEU:HD13	1:B:227:VAL:CG2	2.52	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	351/366 (96%)	340 (97%)	11 (3%)	0	100	100
1	B	363/366 (99%)	358 (99%)	5 (1%)	0	100	100
All	All	714/732 (98%)	698 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	297/313 (95%)	287 (97%)	10 (3%)	37	51
1	B	309/313 (99%)	304 (98%)	5 (2%)	62	78
All	All	606/626 (97%)	591 (98%)	15 (2%)	47	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	70	VAL
1	A	73	ARG
1	A	87	GLU
1	A	120	ASP
1	A	176	ARG
1	A	207	LEU
1	A	212	ASN
1	A	282	ARG
1	A	331	LEU
1	B	39	ASP
1	B	98	LEU
1	B	176	ARG
1	B	251	ASN
1	B	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	123	GLN
1	A	212	ASN
1	A	221	ASN
1	A	255	HIS
1	B	16	GLN
1	B	36	GLN

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Mol	Chain	Res	Type
1	B	186	GLN
1	B	212	ASN
1	B	255	HIS
1	B	348	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 5 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEG	A	403	-	6,6,6	0.44	0	5,5,5	0.30	0
3	PEG	A	405	-	6,6,6	0.47	0	5,5,5	0.29	0
4	PG4	A	410	-	12,12,12	0.47	0	11,11,11	0.22	0
3	PEG	B	405	-	6,6,6	0.45	0	5,5,5	0.30	0
3	PEG	B	409	-	6,6,6	0.44	0	5,5,5	0.29	0
3	PEG	B	403	-	6,6,6	0.47	0	5,5,5	0.30	0
3	PEG	A	408	-	6,6,6	0.46	0	5,5,5	0.25	0
3	PEG	B	408	-	6,6,6	0.44	0	5,5,5	0.26	0
4	PG4	B	402	-	12,12,12	0.46	0	11,11,11	0.27	0
3	PEG	B	414	-	6,6,6	0.43	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEG	B	410	-	6,6,6	0.44	0	5,5,5	0.24	0
3	PEG	A	418	-	6,6,6	0.45	0	5,5,5	0.31	0
4	PG4	A	415	-	12,12,12	0.46	0	11,11,11	0.27	0
4	PG4	A	416	-	12,12,12	0.46	0	11,11,11	0.26	0
4	PG4	B	412	-	12,12,12	0.47	0	11,11,11	0.24	0
2	2J1	A	401	-	17,19,19	2.90	6 (35%)	20,28,28	1.83	7 (35%)
3	PEG	A	414	-	6,6,6	0.44	0	5,5,5	0.28	0
3	PEG	A	406	-	6,6,6	0.44	0	5,5,5	0.28	0
3	PEG	B	407	-	6,6,6	0.43	0	5,5,5	0.32	0
4	PG4	A	404	-	12,12,12	0.48	0	11,11,11	0.26	0
4	PG4	B	404	-	12,12,12	0.48	0	11,11,11	0.24	0
3	PEG	A	412	-	6,6,6	0.46	0	5,5,5	0.19	0
4	PG4	B	411	-	12,12,12	0.49	0	11,11,11	0.19	0
3	PEG	A	413	-	6,6,6	0.45	0	5,5,5	0.24	0
3	PEG	B	413	-	6,6,6	0.44	0	5,5,5	0.27	0
3	PEG	A	402	-	6,6,6	0.46	0	5,5,5	0.27	0
4	PG4	B	401	-	12,12,12	0.48	0	11,11,11	0.21	0
4	PG4	B	406	-	12,12,12	0.47	0	11,11,11	0.24	0
3	PEG	B	416	-	6,6,6	0.48	0	5,5,5	0.25	0
3	PEG	B	415	-	6,6,6	0.42	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	403	-	-	3/4/4/4	-
3	PEG	A	405	-	-	4/4/4/4	-
4	PG4	A	410	-	-	7/10/10/10	-
3	PEG	B	405	-	-	3/4/4/4	-
3	PEG	B	409	-	-	3/4/4/4	-
3	PEG	B	403	-	-	3/4/4/4	-
3	PEG	A	408	-	-	3/4/4/4	-
3	PEG	B	408	-	-	4/4/4/4	-
4	PG4	B	402	-	-	4/10/10/10	-
3	PEG	B	414	-	-	2/4/4/4	-
3	PEG	B	410	-	-	2/4/4/4	-
3	PEG	A	418	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	A	415	-	-	8/10/10/10	-
4	PG4	A	416	-	-	4/10/10/10	-
4	PG4	B	412	-	-	6/10/10/10	-
2	2J1	A	401	-	-	4/4/11/11	0/3/3/3
3	PEG	A	414	-	-	1/4/4/4	-
3	PEG	A	406	-	-	4/4/4/4	-
3	PEG	B	407	-	-	4/4/4/4	-
4	PG4	A	404	-	-	7/10/10/10	-
4	PG4	B	404	-	-	6/10/10/10	-
3	PEG	A	412	-	-	2/4/4/4	-
4	PG4	B	411	-	-	9/10/10/10	-
3	PEG	A	413	-	-	1/4/4/4	-
3	PEG	B	413	-	-	1/4/4/4	-
3	PEG	A	402	-	-	2/4/4/4	-
4	PG4	B	401	-	-	6/10/10/10	-
4	PG4	B	406	-	-	7/10/10/10	-
3	PEG	B	416	-	-	3/4/4/4	-
3	PEG	B	415	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	2J1	C12-C1	7.47	1.49	1.39
2	A	401	2J1	C6-C5	6.43	1.48	1.39
2	A	401	2J1	O1-C13	3.63	1.33	1.22
2	A	401	2J1	O2-C13	-2.70	1.22	1.30
2	A	401	2J1	C1-CL	2.63	1.79	1.73
2	A	401	2J1	C3-C4	2.43	1.49	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	2J1	C2-C3-C4	3.22	122.66	118.26
2	A	401	2J1	C8-C7-C6	-3.16	107.70	112.49
2	A	401	2J1	C1-C12-C13	-3.03	119.84	123.83
2	A	401	2J1	C9-C10-C5	-2.67	109.15	113.53
2	A	401	2J1	C11-C12-C1	2.41	120.67	117.92
2	A	401	2J1	C2-C1-C12	-2.25	120.30	121.91
2	A	401	2J1	C10-C5-N	2.03	127.48	122.39

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	411	PG4	O3-C5-C6-O4
3	B	403	PEG	O2-C3-C4-O4
3	B	408	PEG	O1-C1-C2-O2
3	B	410	PEG	O1-C1-C2-O2
4	B	401	PG4	O1-C1-C2-O2
4	B	406	PG4	O4-C7-C8-O5
4	A	415	PG4	O2-C3-C4-O3
3	B	414	PEG	O2-C3-C4-O4
3	B	415	PEG	O2-C3-C4-O4
3	B	416	PEG	O2-C3-C4-O4
4	A	404	PG4	O4-C7-C8-O5
4	A	416	PG4	O1-C1-C2-O2
3	A	418	PEG	O1-C1-C2-O2
3	B	407	PEG	O2-C3-C4-O4
3	B	410	PEG	O2-C3-C4-O4
2	A	401	2J1	C1-C12-C13-O2
2	A	401	2J1	C1-C12-C13-O1
4	B	412	PG4	O2-C3-C4-O3
3	A	403	PEG	O1-C1-C2-O2
3	A	405	PEG	O1-C1-C2-O2
3	A	405	PEG	O2-C3-C4-O4
3	B	403	PEG	O1-C1-C2-O2
3	B	405	PEG	O2-C3-C4-O4
3	B	408	PEG	O2-C3-C4-O4
3	B	409	PEG	O1-C1-C2-O2
4	A	404	PG4	O1-C1-C2-O2
4	A	410	PG4	O1-C1-C2-O2
4	A	410	PG4	O4-C7-C8-O5
4	B	404	PG4	O4-C7-C8-O5
3	A	406	PEG	O1-C1-C2-O2
3	A	408	PEG	O2-C3-C4-O4
4	B	404	PG4	O3-C5-C6-O4
4	A	415	PG4	C8-C7-O4-C6
3	A	403	PEG	C1-C2-O2-C3
4	B	412	PG4	O1-C1-C2-O2
4	A	410	PG4	C4-C3-O2-C2
4	B	401	PG4	C5-C6-O4-C7
3	A	408	PEG	C1-C2-O2-C3
3	A	413	PEG	C1-C2-O2-C3
4	A	410	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
4	B	406	PG4	C6-C5-O3-C4
4	B	411	PG4	C1-C2-O2-C3
3	B	415	PEG	C4-C3-O2-C2
4	A	415	PG4	C5-C6-O4-C7
4	B	401	PG4	C1-C2-O2-C3
4	B	412	PG4	C6-C5-O3-C4
3	B	409	PEG	C1-C2-O2-C3
4	B	411	PG4	C8-C7-O4-C6
3	A	402	PEG	C1-C2-O2-C3
3	B	403	PEG	C4-C3-O2-C2
4	B	404	PG4	C3-C4-O3-C5
4	B	412	PG4	C8-C7-O4-C6
3	A	402	PEG	C4-C3-O2-C2
3	B	405	PEG	C1-C2-O2-C3
4	B	404	PG4	C8-C7-O4-C6
4	B	402	PG4	C3-C4-O3-C5
4	B	406	PG4	C1-C2-O2-C3
4	B	401	PG4	C4-C3-O2-C2
4	A	410	PG4	C3-C4-O3-C5
3	A	408	PEG	C4-C3-O2-C2
3	A	414	PEG	C1-C2-O2-C3
3	A	418	PEG	C1-C2-O2-C3
3	B	416	PEG	C1-C2-O2-C3
4	A	416	PG4	C3-C4-O3-C5
4	B	406	PG4	C5-C6-O4-C7
4	B	412	PG4	C4-C3-O2-C2
3	B	407	PEG	C1-C2-O2-C3
3	B	407	PEG	C4-C3-O2-C2
3	B	414	PEG	C1-C2-O2-C3
3	A	405	PEG	C4-C3-O2-C2
3	A	403	PEG	C4-C3-O2-C2
4	B	402	PG4	C4-C3-O2-C2
3	B	416	PEG	C4-C3-O2-C2
3	A	406	PEG	C1-C2-O2-C3
4	B	401	PG4	O2-C3-C4-O3
4	A	415	PG4	O1-C1-C2-O2
4	B	402	PG4	O4-C7-C8-O5
4	A	415	PG4	C6-C5-O3-C4
4	A	416	PG4	C1-C2-O2-C3
4	A	404	PG4	C6-C5-O3-C4
3	B	405	PEG	C4-C3-O2-C2
4	A	416	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	A	418	PEG	C4-C3-O2-C2
4	A	404	PG4	C5-C6-O4-C7
4	B	411	PG4	C3-C4-O3-C5
3	B	408	PEG	C1-C2-O2-C3
3	B	413	PEG	C1-C2-O2-C3
4	A	404	PG4	C1-C2-O2-C3
4	B	411	PG4	C4-C3-O2-C2
3	A	406	PEG	O2-C3-C4-O4
4	A	410	PG4	C5-C6-O4-C7
4	B	412	PG4	C5-C6-O4-C7
4	A	404	PG4	C8-C7-O4-C6
4	A	404	PG4	C3-C4-O3-C5
3	B	408	PEG	C4-C3-O2-C2
4	B	401	PG4	C3-C4-O3-C5
4	B	411	PG4	C5-C6-O4-C7
4	B	404	PG4	C4-C3-O2-C2
4	A	415	PG4	C3-C4-O3-C5
2	A	401	2J1	C11-C12-C13-O1
4	B	402	PG4	O2-C3-C4-O3
4	A	410	PG4	C1-C2-O2-C3
2	A	401	2J1	C11-C12-C13-O2
4	B	411	PG4	C6-C5-O3-C4
3	A	406	PEG	C4-C3-O2-C2
4	A	415	PG4	O3-C5-C6-O4
3	A	412	PEG	C1-C2-O2-C3
3	B	409	PEG	C4-C3-O2-C2
4	B	411	PG4	O2-C3-C4-O3
4	A	415	PG4	C4-C3-O2-C2
4	B	404	PG4	O2-C3-C4-O3
3	A	412	PEG	O2-C3-C4-O4
3	B	407	PEG	O1-C1-C2-O2
4	B	411	PG4	O4-C7-C8-O5
3	A	405	PEG	C1-C2-O2-C3
4	B	406	PG4	C8-C7-O4-C6
4	B	406	PG4	O3-C5-C6-O4
4	B	406	PG4	C4-C3-O2-C2

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	410	PG4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	409	PEG	1	0
3	B	408	PEG	1	0
3	B	414	PEG	1	0
3	B	410	PEG	1	0
4	B	412	PG4	2	0
2	A	401	2J1	1	0
4	A	404	PG4	1	0
4	B	404	PG4	1	0
4	B	411	PG4	2	0
4	B	401	PG4	4	0
3	B	416	PEG	1	0
3	B	415	PEG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	356/366 (97%)	0.44	9 (2%)	57	64	13, 21, 29, 37	1 (0%)
1	B	365/366 (99%)	0.45	15 (4%)	37	44	13, 20, 35, 39	0
All	All	721/732 (98%)	0.45	24 (3%)	46	53	13, 20, 31, 39	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	VAL	4.0
1	B	211	ASP	3.5
1	A	284	TYR	3.3
1	B	209	GLY	3.2
1	A	148	HIS	3.1
1	B	253	ASP	3.0
1	B	210	GLY	3.0
1	B	274	SER	2.7
1	B	207	LEU	2.7
1	B	366	LEU	2.7
1	A	201	ILE	2.3
1	B	251	ASN	2.3
1	A	19	GLY	2.3
1	B	156	ASN	2.2
1	B	297	PRO	2.2
1	B	226	HIS	2.2
1	A	253	ASP	2.2
1	A	153	TYR	2.2
1	B	190	SER	2.2
1	A	330	ALA	2.2
1	B	208	ASP	2.0
1	B	204	MET	2.0
1	B	252	PRO	2.0
1	A	251	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	B	416	7/7	0.54	0.34	51,54,56,56	0
4	PG4	B	411	13/13	0.59	0.32	48,50,51,52	0
4	PG4	B	401	13/13	0.64	0.33	37,38,39,39	0
3	PEG	B	408	7/7	0.66	0.34	40,40,41,41	0
3	PEG	B	403	7/7	0.67	0.23	27,27,28,28	0
4	PG4	A	415	13/13	0.67	0.31	46,47,50,50	0
2	2J1	A	401	17/17	0.70	0.23	51,51,52,53	0
3	PEG	B	405	7/7	0.70	0.29	55,56,56,56	0
3	PEG	A	408	7/7	0.70	0.19	29,30,30,30	0
4	PG4	B	406	13/13	0.70	0.23	47,50,51,51	0
3	PEG	B	410	7/7	0.70	0.25	44,44,45,45	0
3	PEG	A	414	7/7	0.72	0.35	58,59,59,59	0
3	PEG	A	405	7/7	0.73	0.25	38,38,38,38	0
3	PEG	B	409	7/7	0.73	0.18	44,45,45,45	0
3	PEG	A	418	7/7	0.75	0.24	51,52,52,52	0
4	PG4	A	404	13/13	0.77	0.23	35,36,38,38	0
3	PEG	B	413	7/7	0.79	0.22	55,55,56,56	0
4	PG4	A	410	13/13	0.79	0.26	28,29,30,30	0
3	PEG	A	413	7/7	0.80	0.19	37,37,38,38	0
5	CA	A	409	1/1	0.80	0.11	58,58,58,58	0
3	PEG	A	402	7/7	0.81	0.19	34,34,34,34	0
4	PG4	A	416	13/13	0.81	0.19	40,41,44,44	0
3	PEG	B	414	7/7	0.82	0.20	38,39,39,40	0
3	PEG	A	406	7/7	0.82	0.17	31,31,31,31	0
4	PG4	B	404	13/13	0.84	0.19	34,35,36,36	0
3	PEG	A	412	7/7	0.84	0.22	28,29,29,29	0
3	PEG	B	407	7/7	0.86	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG4	B	402	13/13	0.86	0.17	30,31,32,32	0
4	PG4	B	412	13/13	0.87	0.18	25,27,27,28	0
3	PEG	A	403	7/7	0.87	0.17	41,41,42,42	0
3	PEG	B	415	7/7	0.92	0.35	21,21,21,22	0
5	CA	B	417	1/1	0.95	0.12	43,43,43,43	0
5	CA	A	417	1/1	0.96	0.10	52,52,52,52	0
5	CA	A	407	1/1	0.98	0.12	31,31,31,31	0
5	CA	A	411	1/1	0.98	0.07	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.