



# Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 02:11 PM BST

PDB ID : 4IIS  
Title : Crystal structure of a glycosylated beta-1,3-glucanase (HEV B 2), An allergen from Hevea Brasiliensis (Space group P41)  
Authors : Rodriguez-Romero, A.; Hernandez-Santoyo, A.  
Deposited on : 2012-12-20  
Resolution : 2.67 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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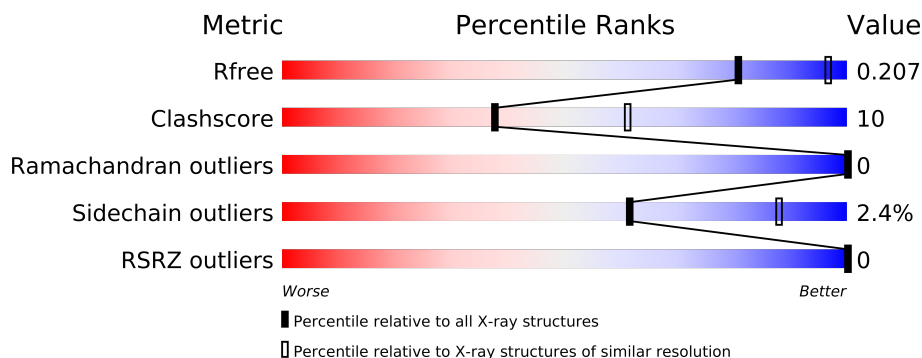
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23004  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 2.67 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))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	316	
1	B	316	
1	C	316	
1	D	316	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CAC	A	403	X	X

## 2 Entry composition i

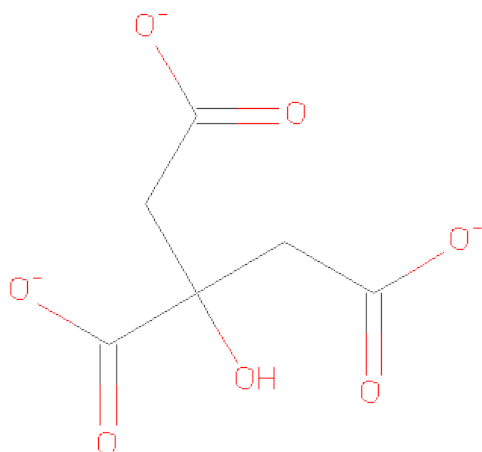
There are 6 unique types of molecules in this entry. The entry contains 10016 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Beta-1,3-glucanase form 'RRII Gln 2'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2466	1586	425	450	5			
1	B	316	Total	C	N	O	S	0	0	0
			2473	1585	428	455	5			
1	C	316	Total	C	N	O	S	0	0	0
			2466	1580	427	454	5			
1	D	316	Total	C	N	O	S	0	0	0
			2482	1592	429	456	5			

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



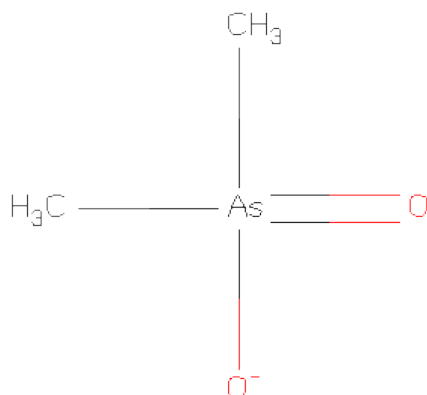
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		

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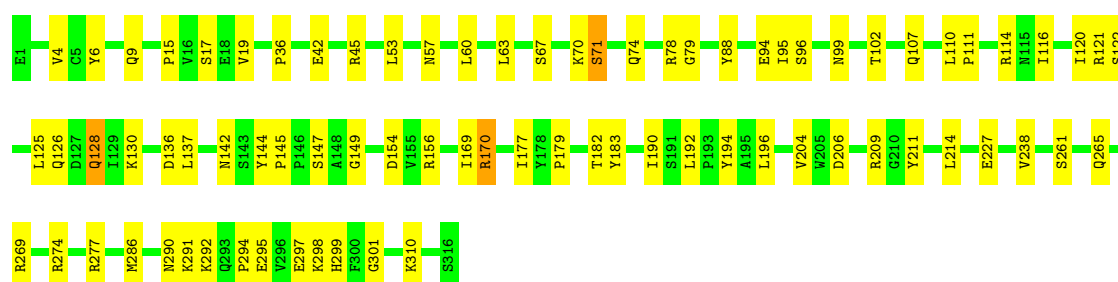
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	11	Total 11	O 11	0	0
6	C	16	Total 16	O 16	0	0
6	D	17	Total 17	O 17	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

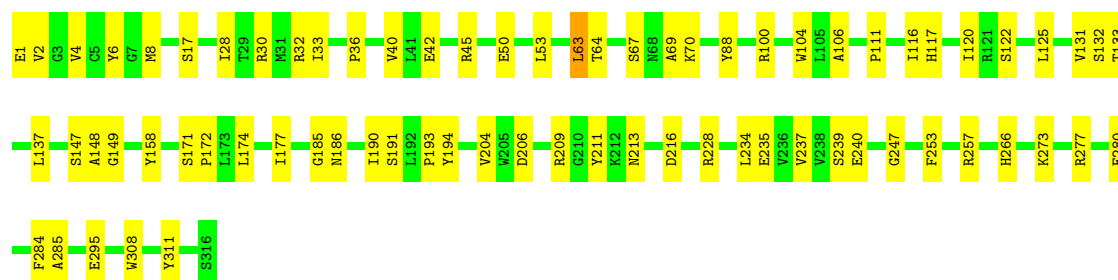
- Molecule 1: Beta-1,3-glucanase form 'RRII Gln 2'

Chain A:



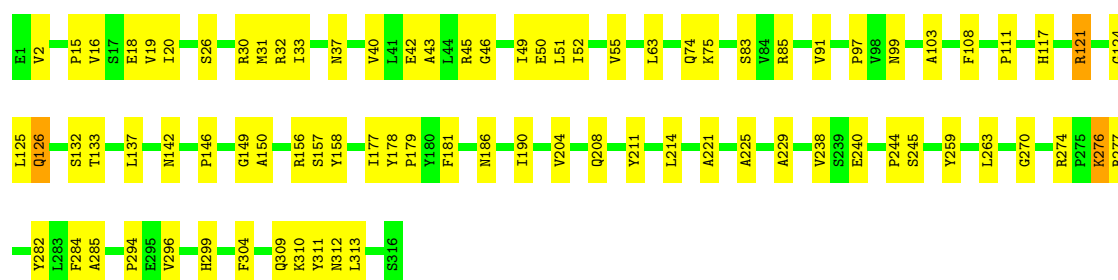
- Molecule 1: Beta-1,3-glucanase form 'RRII Gln 2'

Chain B:



- Molecule 1: Beta-1,3-glucanase form 'RRII Gln 2'

Chain C:



- Molecule 1: Beta-1,3-glucanase form 'RRII Gln 2'

Chain D:

S316	S157	E1
	Y158	V2
	F165	Y6
	I169	Q9
	R170	
	L173	V19
	L174	
	I177	Y23
	Y178	K24
	R188	R30
	D189	M31
	V202	R32
		I33
		Y34
		E42
	W205	
	Y211	R45
	D220	L51
		I52
	A229	L63
	E240	T64
	D254	N65
		P66
		F80
	R257	
	Q265	I95
	H266	
	V267	R100
	K268	G101
		T102
		A103
	K273	W104
		L105
	R277	A106
	T281	I116
	Y282	
	D288	I120
	E289	R121
	N290	S122
	K291	
	K292	L125
	K298	Q128
	F304	S132
		T133
	W308	L137
	Q309	
	K310	Y144
	Y311	
		R156

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.12Å 150.12Å 77.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.47 – 2.67 47.47 – 2.66	Depositor EDS
% Data completeness (in resolution range)	93.5 (47.47-2.67) 93.5 (47.47-2.66)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1380)	Depositor
R, $R_{free}$	0.202 , 0.220 0.198 , 0.207	Depositor DCC
$R_{free}$ test set	2334 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.2	EDS
Estimated twinning fraction	0.500 for h,-k,-l 0.470 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 46212 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, NA, FLC, PCA, NAG

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	0.56	0/2524	0.77	0/3438
1	B	0.55	0/2529	0.79	0/3442
1	C	0.59	0/2522	0.78	0/3435
1	D	0.59	0/2540	0.79	0/3459
All	All	0.57	0/10115	0.78	0/13774

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2466	0	2426	53	0
1	B	2473	0	2443	53	0
1	C	2466	0	2424	63	0
1	D	2482	0	2446	42	0
2	A	26	0	10	1	0
2	D	13	0	5	0	0
3	A	5	0	0	0	0
4	C	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
6	A	12	0	0	1	0
6	B	11	0	0	0	0
6	C	16	0	0	0	0
6	D	17	0	0	0	0
All	All	10016	0	9779	198	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (198) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:174:LEU:HD12	1:B:239:SER:HB3	1.49	0.95
1:C:137:LEU:HD11	1:C:177:ILE:HG12	1.52	0.92
1:C:276:LYS:HD2	1:C:277:ARG:H	1.38	0.86
1:D:188:ARG:NH1	1:D:189:ASP:OD1	2.16	0.78
1:B:204:VAL:HB	1:B:211:TYR:HB2	1.67	0.76
1:C:33:ILE:HG12	1:C:51:LEU:HD11	1.68	0.76
1:D:2:VAL:HG23	1:D:281:THR:HG23	1.67	0.75
1:B:63:LEU:HD12	1:B:116:ILE:HD11	1.70	0.72
1:A:71:SER:HB2	1:B:253:PHE:CD1	2.25	0.71
1:A:227:GLU:OE2	1:A:274:ARG:NH2	2.20	0.71
1:A:107:GLN:CD	1:A:107:GLN:H	1.95	0.69
1:C:126:GLN:H	1:C:126:GLN:CD	1.96	0.69
1:A:182:THR:HB	1:A:214:LEU:HD21	1.75	0.67
1:D:265:GLN:OE1	1:D:268:LYS:NZ	2.25	0.66
1:D:52:ILE:HD13	1:D:174:LEU:HD21	1.78	0.66
1:C:124:GLY:HA2	1:C:126:GLN:HE22	1.60	0.66
1:A:125:LEU:HA	1:A:128:GLN:HE21	1.61	0.66
1:C:74:GLN:OE1	1:D:308:TRP:NE1	2.23	0.66
1:C:309:GLN:NE2	1:C:313:LEU:H	1.95	0.64
1:A:137:LEU:HD11	1:A:177:ILE:HG12	1.80	0.63
1:C:276:LYS:HD2	1:C:277:ARG:N	2.10	0.63
1:C:50:GLU:HG3	1:C:85:ARG:HD3	1.80	0.63
1:A:36:PRO:HB3	1:A:53:LEU:HD11	1.83	0.61
1:C:26:SER:HA	4:C:401:NAG:H82	1.83	0.61
1:D:156:ARG:NH2	1:D:229:ALA:HA	2.16	0.60
1:D:137:LEU:HD11	1:D:177:ILE:HG12	1.84	0.60
1:D:267:VAL:HG11	1:D:281:THR:HG21	1.81	0.60
1:B:149:GLY:O	1:B:228:ARG:NH1	2.35	0.59
1:A:114:ARG:HD3	6:A:507:HOH:O	2.01	0.59
1:A:297:GLU:OE1	1:D:100:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:294:PRO:HG2	1:C:296:VAL:HG12	1.84	0.59
1:B:120:ILE:HG23	1:B:125:LEU:HB2	1.84	0.59
1:A:290:ASN:O	1:A:298:LYS:NZ	2.21	0.58
1:A:183:TYR:CZ	1:A:192:LEU:HG	2.39	0.58
1:C:309:GLN:HE22	1:C:313:LEU:H	1.52	0.57
1:D:33:ILE:HG12	1:D:51:LEU:HD11	1.86	0.57
1:C:186:ASN:O	1:C:190:ILE:HD12	2.04	0.57
1:A:121:ARG:CZ	1:A:126:GLN:HG3	2.35	0.57
1:A:274:ARG:HH11	1:A:277:ARG:HH22	1.54	0.56
1:A:74:GLN:OE1	1:A:78:ARG:HD3	2.04	0.56
1:A:177:ILE:HG22	1:A:179:PRO:HD3	1.87	0.56
1:C:245:SER:HB3	1:C:311:TYR:OH	2.05	0.56
1:B:216:ASP:OD1	1:B:266:HIS:NE2	2.38	0.56
1:B:104:TRP:CZ2	1:C:294:PRO:HG3	2.41	0.56
1:A:294:PRO:HG3	1:D:104:TRP:HZ2	1.71	0.55
1:A:88:TYR:HD1	1:A:130:LYS:HB2	1.72	0.54
1:C:32:ARG:HG3	1:C:52:ILE:HB	1.88	0.54
1:C:146:PRO:O	1:C:221:ALA:HA	2.08	0.54
1:A:96:SER:HB3	1:A:99:ASN:HB2	1.89	0.53
1:B:213:ASN:OD1	1:B:216:ASP:N	2.38	0.53
1:B:132:SER:OG	1:B:133:THR:N	2.42	0.53
1:C:46:GLY:N	1:C:83:SER:HB2	2.24	0.52
1:D:178:TYR:OH	1:D:240:GLU:HB3	2.09	0.52
1:C:177:ILE:HD12	1:C:238:VAL:HG22	1.90	0.52
1:A:261:SER:O	1:A:265:GLN:NE2	2.42	0.52
1:C:309:GLN:CD	1:C:313:LEU:H	2.13	0.52
1:C:126:GLN:N	1:C:126:GLN:OE1	2.43	0.52
1:B:4:VAL:HG21	1:B:28:ILE:HD13	1.91	0.52
1:D:202:VAL:HG21	1:D:205:TRP:CE2	2.45	0.52
1:A:70:LYS:O	1:A:74:GLN:HG2	2.09	0.51
1:A:42:GLU:O	1:A:45:ARG:HG3	2.10	0.51
1:C:30:ARG:HB3	1:C:282:TYR:CE1	2.46	0.51
1:B:137:LEU:HD11	1:B:177:ILE:HG12	1.93	0.51
1:B:191:SER:HB2	1:B:193:PRO:HD2	1.93	0.51
1:D:95:ILE:HG23	1:D:102:THR:HB	1.92	0.51
1:A:67:SER:HA	1:A:70:LYS:HG3	1.92	0.51
1:C:15:PRO:HD2	1:C:18:GLU:OE2	2.10	0.50
1:C:15:PRO:O	1:C:19:VAL:HG23	2.11	0.50
1:A:9:GLN:C	1:A:291:LYS:HD2	2.31	0.50
1:C:16:VAL:HG11	1:C:40:VAL:HA	1.92	0.50
1:A:121:ARG:NH1	1:A:126:GLN:HG3	2.27	0.50
1:C:178:TYR:OH	1:C:240:GLU:HB3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:132:SER:OG	1:C:133:THR:N	2.45	0.50
1:A:274:ARG:HH11	1:A:277:ARG:NH2	2.09	0.49
1:B:64:THR:HG23	1:B:111:PRO:HB2	1.94	0.49
1:D:304:PHE:CZ	1:D:310:LYS:HG2	2.47	0.49
1:B:190:ILE:HG23	1:B:194:TYR:HD2	1.77	0.49
1:C:156:ARG:NH2	1:C:229:ALA:HA	2.27	0.49
1:D:42:GLU:HA	1:D:42:GLU:OE1	2.12	0.49
1:C:270:GLY:HA3	1:C:274:ARG:O	2.11	0.49
1:B:171:SER:O	1:B:234:LEU:HD22	2.12	0.49
1:B:88:TYR:CZ	1:B:237:VAL:HG21	2.48	0.49
1:D:202:VAL:HG21	1:D:205:TRP:NE1	2.28	0.49
1:C:259:TYR:CE2	1:C:263:LEU:HD22	2.47	0.49
1:D:6:TYR:CZ	1:D:19:VAL:HG21	2.47	0.49
1:C:142:ASN:O	1:C:149:GLY:HA2	2.13	0.49
1:A:190:ILE:HG23	1:A:194:TYR:HD2	1.78	0.48
1:D:6:TYR:OH	1:D:19:VAL:HG21	2.14	0.48
1:A:154:ASP:HB3	1:D:144:TYR:HE1	1.78	0.48
1:C:20:ILE:HG23	1:C:49:ILE:HD12	1.95	0.48
1:D:132:SER:OG	1:D:133:THR:N	2.46	0.48
1:B:133:THR:O	1:B:174:LEU:HB2	2.14	0.48
1:C:46:GLY:H	1:C:83:SER:HB2	1.79	0.48
1:C:15:PRO:HD2	1:C:18:GLU:CD	2.34	0.48
1:C:16:VAL:CG1	1:C:40:VAL:HA	2.44	0.48
1:C:204:VAL:HG23	1:C:211:TYR:HB2	1.95	0.48
1:A:204:VAL:HB	1:A:211:TYR:HB2	1.95	0.47
1:D:30:ARG:HB3	1:D:282:TYR:CE1	2.48	0.47
1:C:37:ASN:OD1	1:C:40:VAL:HG23	2.14	0.47
1:B:67:SER:HA	1:B:70:LYS:HE2	1.95	0.47
1:B:42:GLU:HA	1:B:45:ARG:HD2	1.96	0.47
1:B:257:ARG:HB2	1:B:311:TYR:CD1	2.49	0.47
1:D:106:ALA:HB1	1:D:158:TYR:CD1	2.49	0.47
1:D:165:PHE:CE2	1:D:169:ILE:HD13	2.49	0.47
1:C:117:HIS:HE1	1:C:121:ARG:NH1	2.13	0.47
1:D:6:TYR:CE2	1:D:19:VAL:HG11	2.51	0.46
1:A:269:ARG:HA	1:A:269:ARG:HD2	1.79	0.46
1:D:254:ASP:OD1	1:D:257:ARG:NH2	2.48	0.46
1:B:67:SER:HA	1:B:70:LYS:HG3	1.97	0.46
1:D:257:ARG:HB2	1:D:311:TYR:CD1	2.51	0.46
1:D:9:GLN:OE1	1:D:292:LYS:HE3	2.15	0.46
1:A:301:GLY:O	1:A:310:LYS:HD3	2.16	0.46
1:A:125:LEU:O	1:A:128:GLN:HG2	2.15	0.46
1:B:6:TYR:CE1	1:B:8:MET:HG2	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:106:ALA:HB1	1:B:158:TYR:CD1	2.51	0.46
1:B:174:LEU:HA	1:B:174:LEU:HD13	1.81	0.46
1:A:15:PRO:O	1:A:19:VAL:HG23	2.16	0.46
1:A:295:GLU:OE2	1:A:299:HIS:NE2	2.25	0.46
1:C:125:LEU:N	1:C:126:GLN:OE1	2.49	0.45
1:B:88:TYR:CE1	1:B:172:PRO:HG3	2.51	0.45
1:B:63:LEU:HD13	1:B:69:ALA:HA	1.98	0.45
1:B:185:GLY:HA2	1:C:103:ALA:O	2.17	0.45
1:C:99:ASN:O	1:C:103:ALA:N	2.50	0.45
1:C:31:MET:N	1:C:50:GLU:O	2.37	0.44
1:B:117:HIS:HA	1:B:131:VAL:HG21	1.98	0.44
1:A:94:GLU:HG2	1:A:136:ASP:HB3	1.99	0.44
1:D:220:ASP:CG	1:D:273:LYS:HB2	2.37	0.44
1:C:42:GLU:O	1:C:45:ARG:HG3	2.18	0.44
1:B:33:ILE:HG21	1:B:40:VAL:HG11	2.00	0.44
1:A:57:ASN:HA	1:A:60:LEU:HG	2.00	0.44
1:B:1:PCA:O	1:B:30:ARG:NH1	2.51	0.44
1:B:147:SER:HB3	1:B:209:ARG:HH22	1.83	0.44
1:A:6:TYR:CZ	1:A:19:VAL:HG11	2.53	0.43
1:C:179:PRO:HB3	1:C:214:LEU:HD23	2.01	0.43
1:C:75:LYS:HB2	1:D:304:PHE:CZ	2.53	0.43
1:C:244:PRO:HA	1:C:299:HIS:O	2.18	0.43
1:A:169:ILE:O	1:A:170:ARG:HG2	2.18	0.43
1:B:204:VAL:O	1:B:211:TYR:N	2.30	0.43
1:A:88:TYR:CD1	1:A:130:LYS:HB2	2.53	0.43
1:B:88:TYR:CE2	1:B:237:VAL:HG21	2.54	0.43
1:C:97:PRO:HG3	1:C:158:TYR:CB	2.49	0.43
1:C:304:PHE:CE2	1:C:310:LYS:HA	2.54	0.43
1:A:116:ILE:O	1:A:120:ILE:HG12	2.19	0.43
1:B:148:ALA:HA	1:B:228:ARG:HH22	1.84	0.43
1:B:104:TRP:HZ2	1:C:294:PRO:HG3	1.84	0.43
1:B:147:SER:HB3	1:B:209:ARG:NH2	2.34	0.43
1:A:292:LYS:O	1:A:298:LYS:NZ	2.51	0.42
1:D:34:TYR:OH	1:D:240:GLU:OE2	2.33	0.42
1:C:16:VAL:HG12	1:C:43:ALA:CB	2.49	0.42
1:C:309:GLN:HE22	1:C:313:LEU:HG	1.85	0.42
1:C:55:VAL:HB	1:C:91:VAL:HA	2.01	0.42
1:B:247:GLY:HA2	1:B:295:GLU:HG3	2.01	0.42
1:D:116:ILE:O	1:D:120:ILE:HG12	2.19	0.42
1:C:284:PHE:HA	1:C:285:ALA:HA	1.73	0.42
1:A:156:ARG:HH22	2:A:401:FLC:HA2	1.85	0.42
1:B:36:PRO:HB3	1:B:53:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:290:ASN:HA	1:D:298:LYS:HG2	2.01	0.42
1:D:42:GLU:OE1	1:D:80:PHE:HE1	2.03	0.42
1:B:206:ASP:HB3	1:B:209:ARG:HB2	2.02	0.42
1:B:284:PHE:CD1	1:B:285:ALA:HB2	2.55	0.42
1:C:150:ALA:HA	1:C:225:ALA:HA	2.02	0.42
1:B:32:ARG:NH1	1:B:240:GLU:HG3	2.35	0.42
1:C:50:GLU:HA	1:C:85:ARG:HB3	2.02	0.41
1:B:88:TYR:HE2	1:B:280:GLU:OE2	2.03	0.41
1:A:6:TYR:OH	1:A:19:VAL:HG21	2.20	0.41
1:A:110:LEU:HB3	1:A:111:PRO:HD3	2.02	0.41
1:A:144:TYR:HA	1:A:145:PRO:HA	1.84	0.41
1:A:79:GLY:HA2	1:B:308:TRP:CD2	2.54	0.41
1:B:172:PRO:HB3	1:B:235:GLU:CG	2.49	0.41
1:B:209:ARG:HH11	1:B:273:LYS:HG3	1.85	0.41
1:B:284:PHE:HA	1:B:285:ALA:HA	1.78	0.41
1:A:147:SER:N	1:A:206:ASP:OD2	2.51	0.41
1:C:108:PHE:C	1:C:111:PRO:HD2	2.41	0.41
1:C:74:GLN:HE21	1:C:74:GLN:HB2	1.68	0.41
1:C:309:GLN:HE22	1:C:313:LEU:N	2.18	0.41
1:D:288:ASP:OD1	1:D:310:LYS:NZ	2.49	0.41
1:B:172:PRO:HB3	1:B:235:GLU:HG3	2.03	0.41
1:B:185:GLY:HA3	1:C:97:PRO:O	2.20	0.41
1:D:125:LEU:HA	1:D:128:GLN:OE1	2.21	0.41
1:C:309:GLN:HB3	1:C:312:ASN:H	1.85	0.41
1:A:177:ILE:HD12	1:A:238:VAL:HG22	2.03	0.41
1:C:186:ASN:HB3	1:C:190:ILE:HD12	2.03	0.41
1:D:211:TYR:OH	1:D:220:ASP:OD2	2.27	0.41
1:B:277:ARG:HA	1:B:277:ARG:HD2	1.79	0.41
1:A:74:GLN:CD	1:A:78:ARG:HD3	2.41	0.41
1:A:206:ASP:N	1:A:209:ARG:O	2.38	0.41
1:D:173:LEU:HA	1:D:173:LEU:HD12	1.85	0.41
1:D:254:ASP:HA	1:D:257:ARG:HH21	1.86	0.40
1:A:142:ASN:O	1:A:149:GLY:HA2	2.22	0.40
1:B:30:ARG:HG2	1:B:50:GLU:HB2	2.02	0.40
1:A:95:ILE:HD13	1:A:102:THR:HB	2.03	0.40
1:D:65:ASN:HA	1:D:66:PRO:HD3	1.93	0.40
1:A:192:LEU:HD22	1:A:196:LEU:HD11	2.04	0.40
1:D:290:ASN:O	1:D:298:LYS:HE2	2.21	0.40
1:B:100:ARG:HG3	1:C:181:PHE:CZ	2.56	0.40
1:A:4:VAL:HG11	1:A:286:MET:SD	2.62	0.40
1:D:23:TYR:CZ	1:D:31:MET:HE2	2.57	0.40
1:B:186:ASN:HD21	1:C:157:SER:HB2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	314/316 (99%)	307 (98%)	7 (2%)	0	100	100
1	B	314/316 (99%)	308 (98%)	6 (2%)	0	100	100
1	C	314/316 (99%)	308 (98%)	6 (2%)	0	100	100
1	D	314/316 (99%)	306 (98%)	8 (2%)	0	100	100
All	All	1256/1264 (99%)	1229 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	260/268 (97%)	254 (98%)	6 (2%)	63	88
1	B	264/268 (98%)	260 (98%)	4 (2%)	76	94
1	C	262/268 (98%)	256 (98%)	6 (2%)	63	88
1	D	265/268 (99%)	256 (97%)	9 (3%)	49	79
All	All	1051/1072 (98%)	1026 (98%)	25 (2%)	61	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	63	LEU
1	A	71	SER

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Mol	Chain	Res	Type
1	A	122	SER
1	A	128	GLN
1	A	170	ARG
1	B	2	VAL
1	B	17	SER
1	B	63	LEU
1	B	122	SER
1	C	2	VAL
1	C	63	LEU
1	C	121	ARG
1	C	126	GLN
1	C	208	GLN
1	C	276	LYS
1	D	2	VAL
1	D	24	LYS
1	D	45	ARG
1	D	63	LEU
1	D	122	SER
1	D	170	ARG
1	D	257	ARG
1	D	277	ARG
1	D	316	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	B	186	ASN
1	B	293	GLN
1	C	74	GLN
1	C	117	HIS
1	C	309	GLN
1	D	76	ASN
1	D	107	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.



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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PCA	A	1	1	8,8,9	6.61	2 (25%)	8,10,12	6.16	4 (50%)
1	PCA	B	1	1	8,8,9	7.13	3 (37%)	8,10,12	7.67	3 (37%)
1	PCA	C	1	1	8,8,9	6.61	3 (37%)	8,10,12	5.32	4 (50%)
1	PCA	D	1	1	8,8,9	7.69	3 (37%)	8,10,12	5.63	4 (50%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	PCA	O-C	20.40	1.25	1.11
1	B	1	PCA	O-C	18.59	1.24	1.11
1	C	1	PCA	O-C	17.62	1.23	1.11
1	A	1	PCA	O-C	17.57	1.23	1.11
1	B	1	PCA	CD-N	6.87	1.49	1.34
1	D	1	PCA	CD-N	6.56	1.48	1.34
1	A	1	PCA	CD-N	6.06	1.47	1.34
1	C	1	PCA	CD-N	5.70	1.46	1.34
1	D	1	PCA	CA-C	3.53	1.55	1.48
1	B	1	PCA	CA-C	3.47	1.54	1.48
1	C	1	PCA	CA-C	2.49	1.52	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	C-CA-N	16.61	114.47	110.71
1	A	1	PCA	CA-N-CD	-15.04	102.62	114.37
1	D	1	PCA	CA-N-CD	-15.03	102.62	114.37
1	C	1	PCA	CA-N-CD	-14.10	103.35	114.37
1	B	1	PCA	CA-N-CD	-13.07	104.16	114.37
1	A	1	PCA	C-CA-N	7.24	112.35	110.71
1	B	1	PCA	OE-CD-CG	-3.75	120.82	126.70
1	A	1	PCA	OE-CD-CG	-3.60	121.05	126.70
1	D	1	PCA	OE-CD-CG	-3.53	121.15	126.70
1	A	1	PCA	CB-CA-N	2.81	111.80	103.72
1	C	1	PCA	OE-CD-CG	-2.71	122.45	126.70
1	C	1	PCA	CB-CA-N	2.69	111.47	103.72
1	D	1	PCA	CB-CA-N	2.52	110.97	103.72
1	C	1	PCA	C-CA-N	2.22	111.22	110.71
1	D	1	PCA	CG-CD-N	2.02	115.03	107.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

2 carbohydrates 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	$\# Z  > 2$
4	NAG	C	401	1,4	12,14,15	0.49	0	15,19,21	0.84	1 (6%)
4	NAG	C	402	4	12,14,15	0.34	0	15,19,21	0.76	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
4	NAG	C	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	402	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	NAG	C3-C2-N2	-2.12	108.53	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
2	FLC	A	401	-	5,12,12	2.99	3 (60%)	7,17,17	1.91	1 (14%)
2	FLC	A	402	-	5,12,12	2.47	4 (80%)	7,17,17	1.49	2 (28%)
3	CAC	A	403	-	4,4,4	4.24	4 (100%)	6,6,6	12.13	3 (50%)
2	FLC	D	401	-	5,12,12	2.22	2 (40%)	7,17,17	2.03	2 (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	FLC	A	401	-	-	0/6/16/16	0/0/0/0
2	FLC	A	402	-	-	0/6/16/16	0/0/0/0
3	CAC	A	403	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	D	401	-	-	0/6/16/16	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	CAC	O2-AS	6.10	1.75	1.68
2	A	401	FLC	CG-CGC	5.47	1.53	1.49
3	A	403	CAC	AS-C1	3.87	1.97	1.90
3	A	403	CAC	AS-C2	3.66	1.96	1.90
2	D	401	FLC	CG-CGC	3.01	1.51	1.49
2	A	402	FLC	CA-CB	-2.94	1.50	1.54
2	D	401	FLC	CA-CB	-2.80	1.50	1.54
2	A	402	FLC	CG-CGC	2.76	1.51	1.49
3	A	403	CAC	O1-AS	2.53	1.75	1.66
2	A	402	FLC	OHB-CB	-2.43	1.39	1.43
2	A	401	FLC	CA-CB	-2.19	1.51	1.54
2	A	402	FLC	CA-CAC	2.18	1.51	1.49
2	A	401	FLC	OHB-CB	-2.01	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	CAC	O2-AS-O1	-28.86	106.31	112.54
3	A	403	CAC	O2-AS-C1	5.50	113.66	109.15
2	D	401	FLC	CB-CA-CAC	-4.42	108.40	115.01
2	A	401	FLC	CB-CA-CAC	-4.38	108.46	115.01
3	A	403	CAC	O2-AS-C2	4.23	112.62	109.15
2	D	401	FLC	CA-CB-CBC	-2.74	105.68	111.21
2	A	402	FLC	CG-CB-CA	-2.61	103.36	109.61
2	A	402	FLC	CB-CA-CAC	2.07	118.09	115.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	316/316 (100%)	-0.07	0 100 100	41, 55, 67, 73	0
1	B	316/316 (100%)	-0.04	0 100 100	36, 56, 71, 80	0
1	C	316/316 (100%)	-0.10	0 100 100	43, 55, 66, 77	0
1	D	316/316 (100%)	-0.03	0 100 100	43, 55, 69, 79	0
All	All	1264/1264 (100%)	-0.06	0 100 100	36, 55, 68, 80	0

There are no RSRZ outliers to report.

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	D	1	8/9	0.19	0.69	57,63,65,67	0
1	PCA	B	1	8/9	0.19	0.16	58,61,63,63	0
1	PCA	A	1	8/9	0.15	-0.37	52,54,56,57	0
1	PCA	C	1	8/9	0.16	-0.64	57,59,64,64	0

### 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	401	14/15	0.19	0.22	65,71,76,79	0
4	NAG	C	402	14/15	0.12	-	59,71,72,75	0

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CAC	A	403	5/5	0.21	2.10	52,54,56,66	0
2	FLC	A	402	13/13	0.16	0.21	55,59,64,65	0
2	FLC	A	401	13/13	0.17	0.14	52,61,71,76	0
2	FLC	D	401	13/13	0.12	-2.08	52,60,64,64	0
5	NA	C	403	1/1	0.13	-33.00	28,28,28,28	0

## 6.5 Other polymers

There are no such residues in this entry.