



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4G5S  
Title : Structure of LGN GL3/Galphai3 complex  
Authors : Jia, M.; Li, J.; Zhu, J.; Wen, W.; Zhang, M.; Wang, W.  
Deposited on : 2012-07-18  
Resolution : 3.62 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

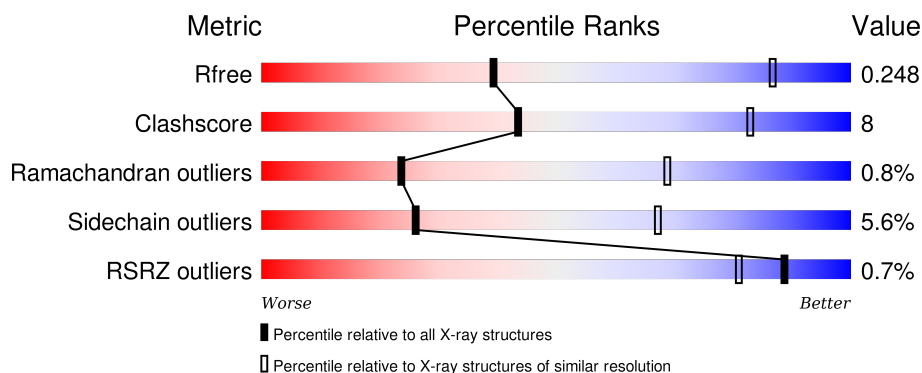
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.62 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))
$R_{free}$	91344	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)

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. 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  $\leq 5\%$ . 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	330	<div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	B	330	<div> <div>%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	C	330	<div> <div>75%</div> <div>19%</div> <div>• 6%</div> </div>
1	D	330	<div> <div>%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	E	25	<div> <div>56%</div> <div>16%</div> <div>8%</div> <div>8%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	25	<div><div></div><div>48%</div><div>20%</div><div>16%</div><div></div><div>12%</div></div>
2	G	25	<div><div>4%</div><div></div><div>60%</div><div>20%</div><div></div><div>16%</div></div>
2	Z	25	<div><div>12%</div><div></div><div>56%</div><div>16%</div><div></div><div>24%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10226 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.

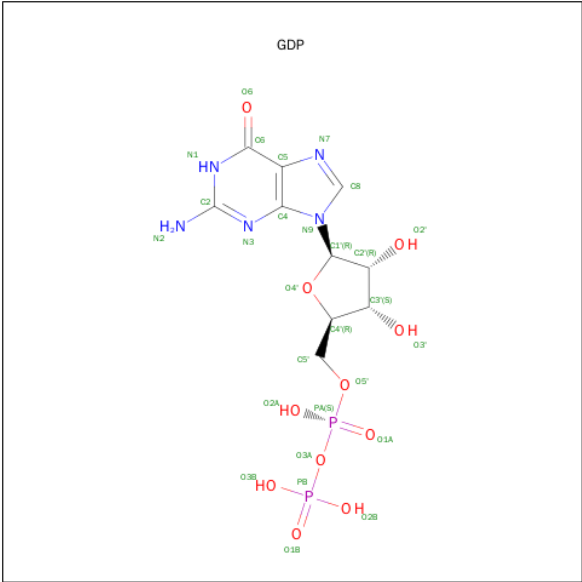
- Molecule 1 is a protein called Guanine nucleotide-binding protein G(k) subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2397	1527	393	463	14			
1	B	316	Total	C	N	O	S	0	0	0
			2359	1500	389	456	14			
1	C	311	Total	C	N	O	S	0	0	0
			2306	1476	373	442	15			
1	D	316	Total	C	N	O	S	0	0	0
			2397	1533	394	454	16			

- Molecule 2 is a protein called G-protein-signaling modulator 2.

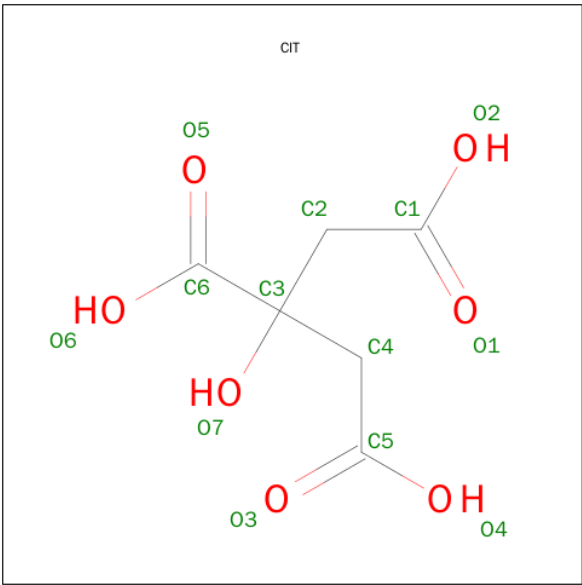
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	22	Total	C	N	O	S	0	0	0
			173	108	30	33	2			
2	G	21	Total	C	N	O	S	0	0	0
			167	104	29	32	2			
2	Z	19	Total	C	N	O	S	0	0	0
			142	88	26	26	2			
2	F	22	Total	C	N	O	S	0	0	0
			175	109	31	33	2			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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

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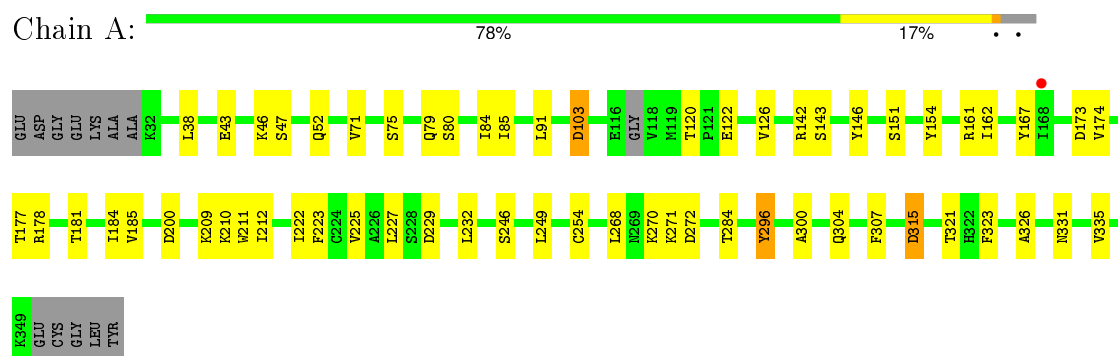
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	6	7		

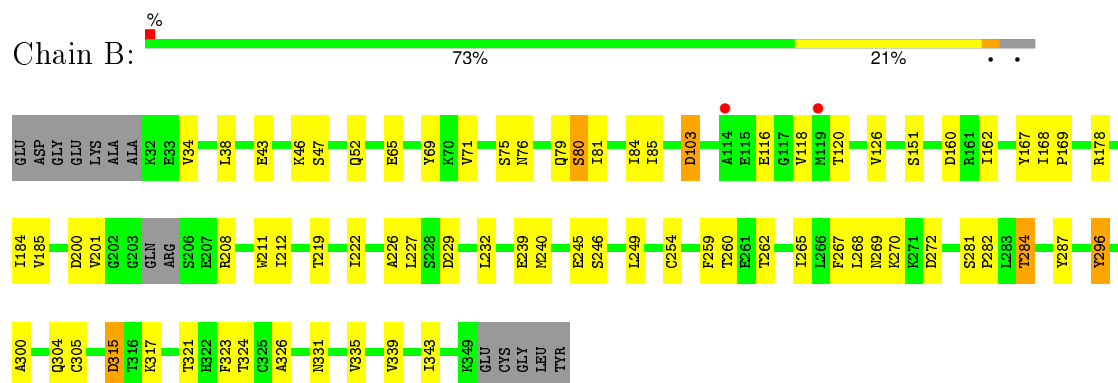
### 3 Residue-property plots

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.

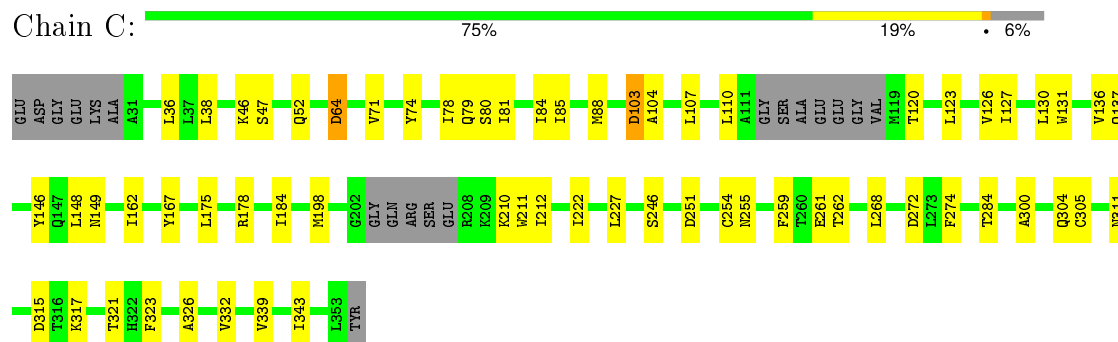
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha



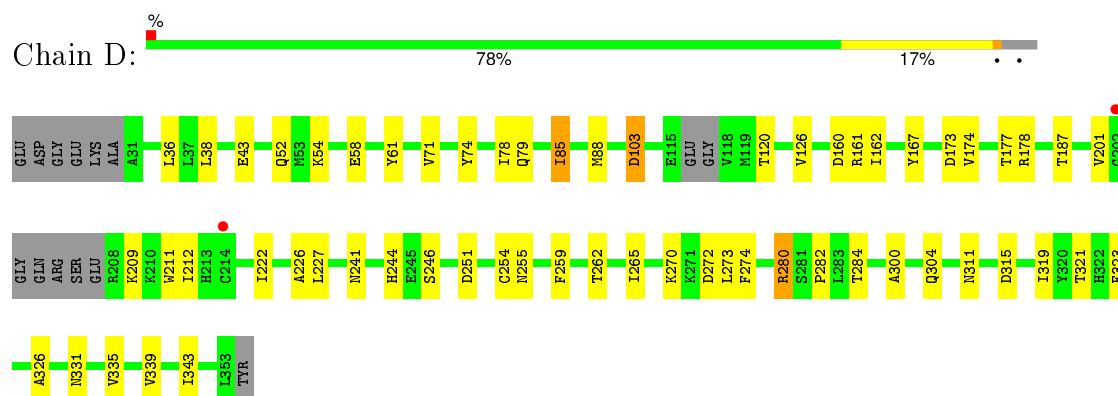
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha



- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha



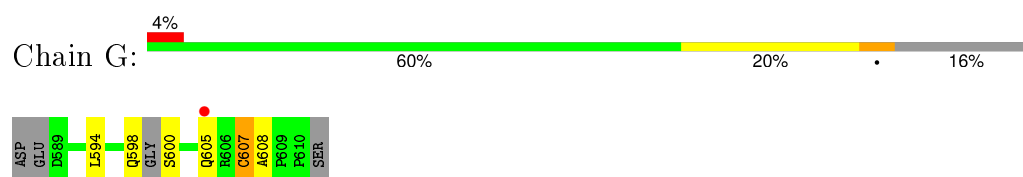
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha



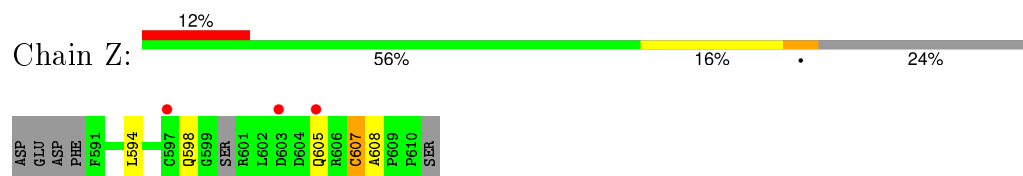
- Molecule 2: G-protein-signaling modulator 2



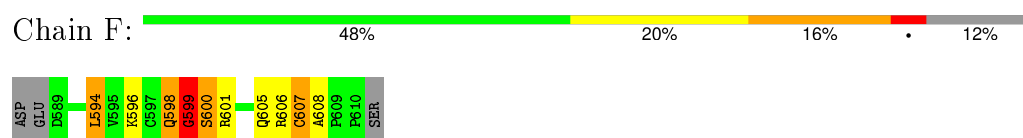
- Molecule 2: G-protein-signaling modulator 2



- Molecule 2: G-protein-signaling modulator 2



- Molecule 2: G-protein-signaling modulator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.68Å 209.68Å 235.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.63 – 3.62 39.63 – 3.62	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.63-3.62) 94.5 (39.63-3.62)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.83 (at 3.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1063)	Depositor
R, $R_{free}$	0.207 , 0.253 0.200 , 0.248	Depositor DCC
$R_{free}$ test set	1675 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	119.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 97.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 35083 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GDP, CIT

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	0.25	0/2440	0.46	0/3320
1	B	0.26	0/2399	0.47	0/3264
1	C	0.25	0/2346	0.46	0/3198
1	D	0.26	0/2440	0.46	0/3314
2	E	0.26	0/176	0.70	1/237 (0.4%)
2	F	0.27	0/178	0.69	1/239 (0.4%)
2	G	0.26	0/169	0.56	0/227
2	Z	0.23	0/143	0.65	0/192
All	All	0.25	0/10291	0.48	2/13991 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	599	GLY	N-CA-C	5.32	126.40	113.10
2	E	599	GLY	N-CA-C	5.15	125.97	113.10

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	2397	0	2226	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2359	0	2192	46	0
1	C	2306	0	2118	35	0
1	D	2397	0	2255	31	0
2	E	173	0	160	7	0
2	F	175	0	167	8	0
2	G	167	0	152	2	0
2	Z	142	0	131	2	0
3	A	28	0	12	4	0
3	B	28	0	12	6	0
3	C	28	0	12	2	0
4	A	13	0	5	1	0
4	C	13	0	5	0	0
All	All	10226	0	9447	160	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 8.

All (160) 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:C:304:GLN:HG3	1:C:321:THR:HG21	1.63	0.78
1:C:103:ASP:HB3	1:C:126:VAL:HG13	1.71	0.72
1:A:103:ASP:HB3	1:A:126:VAL:HG13	1.73	0.70
1:D:103:ASP:HB3	1:D:126:VAL:HG13	1.73	0.70
1:A:271:LYS:NZ	4:A:402:CIT:O5	2.24	0.70
1:D:304:GLN:HG3	1:D:321:THR:HG21	1.73	0.70
1:C:52:GLN:NE2	1:C:326:ALA:O	2.26	0.68
1:A:225:VAL:HG21	1:A:307:PHE:HE2	1.59	0.68
2:E:598:GLN:O	2:E:600:SER:N	2.25	0.67
1:B:304:GLN:HG3	1:B:321:THR:HG21	1.76	0.66
2:F:598:GLN:O	2:F:600:SER:N	2.25	0.65
1:A:227:LEU:HD21	1:A:268:LEU:HB3	1.79	0.64
1:C:64:ASP:OD1	1:C:64:ASP:N	2.28	0.64
1:D:251:ASP:OD1	1:D:255:ASN:ND2	2.30	0.64
1:D:52:GLN:NE2	1:D:326:ALA:O	2.32	0.62
1:A:225:VAL:HG21	1:A:307:PHE:CE2	2.33	0.62
1:A:304:GLN:HG3	1:A:321:THR:HG21	1.82	0.62
1:D:85:ILE:HA	1:D:88:MET:HE2	1.81	0.62
1:B:103:ASP:HB3	1:B:126:VAL:HG13	1.82	0.61
1:B:184:ILE:HD11	1:B:211:TRP:HA	1.83	0.61
1:A:209:LYS:HA	1:C:261:GLU:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLN:NE2	1:A:326:ALA:O	2.34	0.60
1:B:240:MET:HG3	1:B:245:GLU:HG3	1.81	0.60
1:B:211:TRP:HE3	1:B:212:ILE:HG12	1.67	0.58
1:A:47:SER:OG	3:A:401:GDP:O2A	2.20	0.58
1:B:43:GLU:OE1	1:B:178:ARG:NH1	2.37	0.57
1:C:300:ALA:HB1	1:C:323:PHE:CE2	2.40	0.56
1:B:76:ASN:O	1:B:80:SER:OG	2.23	0.56
1:B:262:THR:O	1:B:317:LYS:NZ	2.35	0.56
1:C:110:LEU:HD13	1:C:123:LEU:HD22	1.88	0.56
1:A:38:LEU:HD23	1:A:222:ILE:HB	1.88	0.56
1:C:47:SER:OG	3:C:401:GDP:O2A	2.23	0.55
1:B:52:GLN:NE2	1:B:326:ALA:O	2.39	0.55
1:C:46:LYS:NZ	3:C:401:GDP:O2B	2.36	0.55
1:B:227:LEU:HD21	1:B:268:LEU:HB3	1.89	0.54
1:B:315:ASP:N	1:B:315:ASP:OD1	2.38	0.53
2:G:607:CYS:SG	2:G:608:ALA:N	2.82	0.53
2:Z:607:CYS:SG	2:Z:608:ALA:N	2.82	0.53
1:A:315:ASP:OD1	1:A:315:ASP:N	2.42	0.52
2:E:607:CYS:SG	2:E:608:ALA:N	2.82	0.52
1:D:300:ALA:HB1	1:D:323:PHE:CE2	2.45	0.51
1:C:300:ALA:HB1	1:C:323:PHE:HE2	1.75	0.51
1:C:38:LEU:HD23	1:C:222:ILE:HB	1.91	0.51
1:B:265:ILE:HD13	1:B:339:VAL:HG13	1.92	0.51
1:A:151:SER:OG	3:A:401:GDP:O3'	2.22	0.51
1:B:272:ASP:OD1	1:B:272:ASP:N	2.44	0.51
1:C:52:GLN:HG2	1:C:332:VAL:HG21	1.92	0.50
1:B:249:LEU:HD11	2:F:594:LEU:HD22	1.94	0.50
1:B:47:SER:OG	3:B:401:GDP:O2A	2.29	0.50
1:D:38:LEU:HD23	1:D:222:ILE:HB	1.93	0.50
1:D:300:ALA:HB1	1:D:323:PHE:HE2	1.77	0.49
1:D:209:LYS:C	1:D:211:TRP:H	2.14	0.49
1:A:272:ASP:OD1	1:A:272:ASP:N	2.45	0.49
1:C:80:SER:O	1:C:84:ILE:HG13	2.12	0.49
1:A:185:VAL:HB	1:A:200:ASP:HB3	1.95	0.48
1:B:151:SER:HG	3:B:401:GDP:HO3'	1.60	0.48
1:D:265:ILE:HD13	1:D:339:VAL:HG13	1.95	0.48
1:D:272:ASP:N	1:D:272:ASP:OD1	2.47	0.48
1:A:154:TYR:OH	1:A:173:ASP:OD1	2.25	0.48
1:C:79:GLN:HB3	2:G:605:GLN:HA	1.94	0.48
1:C:162:ILE:HG22	1:C:167:TYR:CZ	2.48	0.48
1:B:38:LEU:HD23	1:B:222:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:607:CYS:SG	2:F:608:ALA:N	2.86	0.48
1:D:54:LYS:HG2	1:D:61:TYR:CE1	2.48	0.48
1:B:80:SER:O	1:B:84:ILE:HG13	2.13	0.48
1:D:227:LEU:HB3	1:D:274:PHE:CD2	2.49	0.48
1:B:185:VAL:HB	1:B:200:ASP:HB3	1.96	0.47
1:B:208:ARG:O	1:B:212:ILE:HG13	2.15	0.47
1:B:259:PHE:HB3	1:B:262:THR:HB	1.97	0.47
1:C:127:ILE:HA	1:C:130:LEU:HD12	1.97	0.47
1:A:296:TYR:CD1	1:A:296:TYR:C	2.88	0.47
1:B:79:GLN:OE1	2:F:606:ARG:N	2.48	0.47
1:B:201:VAL:HG13	1:B:211:TRP:NE1	2.30	0.47
1:C:251:ASP:OD1	1:C:255:ASN:ND2	2.48	0.47
1:C:311:ASN:ND2	1:C:317:LYS:O	2.48	0.47
1:C:184:ILE:HD11	1:C:211:TRP:HA	1.97	0.47
1:C:131:TRP:O	1:C:137:GLN:NE2	2.47	0.46
1:A:79:GLN:OE1	2:E:606:ARG:N	2.48	0.46
1:D:339:VAL:O	1:D:343:ILE:HG13	2.16	0.46
1:C:272:ASP:N	1:C:272:ASP:OD1	2.47	0.46
1:D:43:GLU:OE2	1:D:178:ARG:NH1	2.49	0.46
1:D:103:ASP:N	1:D:103:ASP:OD1	2.49	0.46
1:A:43:GLU:OE2	1:A:178:ARG:NH1	2.48	0.46
3:B:401:GDP:O3B	2:F:601:ARG:NH1	2.49	0.46
1:B:296:TYR:CD1	1:B:296:TYR:C	2.89	0.46
1:B:46:LYS:NZ	3:B:401:GDP:O2B	2.28	0.45
1:B:75:SER:O	1:B:79:GLN:HG3	2.16	0.45
1:B:269:ASN:ND2	3:B:401:GDP:N7	2.65	0.45
1:A:296:TYR:HD1	1:A:296:TYR:C	2.20	0.45
1:B:34:VAL:HG13	1:B:219:THR:HG21	1.97	0.45
1:B:151:SER:OG	3:B:401:GDP:O3'	2.32	0.45
1:A:331:ASN:O	1:A:335:VAL:HG23	2.16	0.45
1:A:46:LYS:NZ	3:A:401:GDP:O2B	2.42	0.45
1:B:81:ILE:HA	1:B:84:ILE:HD12	1.98	0.45
1:D:241:ASN:OD1	1:D:244:HIS:ND1	2.40	0.45
1:A:229:ASP:HA	1:A:232:LEU:HG	1.98	0.45
1:C:227:LEU:HD21	1:C:268:LEU:HB3	1.99	0.45
1:A:43:GLU:OE2	2:E:606:ARG:NH1	2.50	0.44
1:B:116:GLU:OE2	1:B:116:GLU:N	2.50	0.44
1:A:122:GLU:O	1:A:126:VAL:HG23	2.17	0.44
1:A:103:ASP:N	1:A:103:ASP:OD1	2.51	0.44
1:B:103:ASP:N	1:B:103:ASP:OD1	2.51	0.44
1:A:174:VAL:HA	1:A:177:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLU:OE2	1:D:187:THR:OG1	2.37	0.43
1:D:259:PHE:HB3	1:D:262:THR:HB	1.99	0.43
1:C:88:MET:SD	1:C:136:VAL:HG22	2.59	0.43
1:C:81:ILE:HA	1:C:84:ILE:HD12	2.00	0.43
1:C:227:LEU:HB3	1:C:274:PHE:CD2	2.54	0.43
1:C:74:TYR:O	1:C:78:ILE:HG13	2.19	0.43
1:B:331:ASN:O	1:B:335:VAL:HG23	2.19	0.43
1:B:65:GLU:O	1:B:69:TYR:HD1	2.01	0.43
1:D:43:GLU:OE1	1:D:178:ARG:NH1	2.52	0.43
1:A:80:SER:O	1:A:84:ILE:HG13	2.19	0.43
1:B:178:ARG:NH2	2:F:605:GLN:O	2.51	0.43
1:A:184:ILE:HD11	1:A:211:TRP:HA	2.02	0.42
1:A:270:LYS:HG2	3:A:401:GDP:C5	2.54	0.42
1:D:36:LEU:HD23	1:D:36:LEU:HA	1.85	0.42
1:A:223:PHE:HE2	1:A:249:LEU:HG	1.84	0.42
1:D:280:ARG:O	1:D:282:PRO:HD3	2.19	0.42
1:A:91:LEU:HB3	1:A:142:ARG:HH11	1.85	0.42
1:D:174:VAL:HA	1:D:177:THR:HG23	2.00	0.42
1:C:146:TYR:CE2	1:C:148:LEU:HB2	2.54	0.42
1:A:75:SER:O	1:A:79:GLN:HG3	2.19	0.42
1:B:284:THR:HA	1:B:287:TYR:O	2.20	0.42
1:D:79:GLN:CB	2:Z:605:GLN:HA	2.50	0.42
1:A:143:SER:HA	1:A:146:TYR:CE1	2.55	0.42
1:B:168:ILE:HA	1:B:169:PRO:HD3	1.83	0.42
2:E:598:GLN:HB3	2:E:599:GLY:H	1.60	0.41
1:D:161:ARG:HH22	1:D:173:ASP:CG	2.23	0.41
1:B:300:ALA:HB1	1:B:323:PHE:CE2	2.55	0.41
1:A:162:ILE:HG22	1:A:167:TYR:CE1	2.55	0.41
1:D:270:LYS:HB3	1:D:273:LEU:HD12	2.01	0.41
1:A:300:ALA:HB1	1:A:323:PHE:CE2	2.55	0.41
1:A:79:GLN:HB3	2:E:605:GLN:HA	2.03	0.41
1:C:339:VAL:O	1:C:343:ILE:HG13	2.21	0.41
1:A:161:ARG:HH22	1:A:173:ASP:CG	2.24	0.41
1:B:229:ASP:HA	1:B:232:LEU:HG	2.02	0.41
1:D:74:TYR:O	1:D:78:ILE:HG13	2.21	0.41
1:B:267:PHE:CD2	1:B:324:THR:HG21	2.55	0.41
1:C:36:LEU:CB	1:C:198:MET:HG3	2.51	0.41
1:D:311:ASN:HB2	1:D:319:ILE:HD11	2.03	0.41
1:C:103:ASP:OD1	1:C:103:ASP:N	2.54	0.41
1:B:162:ILE:HG22	1:B:167:TYR:CZ	2.56	0.41
1:C:259:PHE:HB3	1:C:262:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:HB2	1:C:178:ARG:NE	2.36	0.41
1:B:281:SER:HA	1:B:282:PRO:HD3	1.94	0.41
1:D:162:ILE:HG22	1:D:167:TYR:CZ	2.55	0.41
1:C:146:TYR:HE2	1:C:148:LEU:HB2	1.86	0.41
1:C:52:GLN:OE1	1:C:175:LEU:HD11	2.21	0.40
2:F:598:GLN:HB3	2:F:599:GLY:H	1.67	0.40
1:C:104:ALA:O	1:C:107:LEU:HB3	2.21	0.40
1:B:339:VAL:O	1:B:343:ILE:HG13	2.22	0.40
1:B:162:ILE:HG22	1:B:167:TYR:CE1	2.56	0.40
1:B:239:GLU:OE2	2:F:596:LYS:HD2	2.21	0.40
1:A:209:LYS:O	1:A:212:ILE:N	2.44	0.40
1:A:178:ARG:NH2	2:E:605:GLN:O	2.53	0.40
1:B:226:ALA:HB1	1:B:270:LYS:HD2	2.04	0.40
1:D:331:ASN:O	1:D:335:VAL:HG23	2.21	0.40
1:A:209:LYS:O	1:A:211:TRP:N	2.54	0.40
1:D:226:ALA:HB1	1:D:270:LYS:HD2	2.03	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	313/330 (95%)	301 (96%)	11 (4%)	1 (0%)	46	83
1	B	312/330 (94%)	299 (96%)	13 (4%)	0	100	100
1	C	305/330 (92%)	293 (96%)	10 (3%)	2 (1%)	26	72
1	D	310/330 (94%)	297 (96%)	11 (4%)	2 (1%)	30	74
2	E	20/25 (80%)	16 (80%)	2 (10%)	2 (10%)	1	11
2	F	20/25 (80%)	16 (80%)	2 (10%)	2 (10%)	1	11
2	G	17/25 (68%)	16 (94%)	1 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	15/25 (60%)	13 (87%)	1 (7%)	1 (7%)	1	22
All	All	1312/1420 (92%)	1251 (95%)	51 (4%)	10 (1%)	24	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	LYS
1	C	210	LYS
1	D	201	VAL
1	D	315	ASP
2	E	599	GLY
2	F	599	GLY
2	E	598	GLN
2	Z	598	GLN
2	F	598	GLN
1	C	315	ASP

### 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	242/290 (83%)	232 (96%)	10 (4%)	37	75
1	B	237/290 (82%)	223 (94%)	14 (6%)	24	66
1	C	227/290 (78%)	217 (96%)	10 (4%)	35	74
1	D	243/290 (84%)	233 (96%)	10 (4%)	37	75
2	E	19/23 (83%)	15 (79%)	4 (21%)	1	10
2	F	20/23 (87%)	17 (85%)	3 (15%)	3	25
2	G	19/23 (83%)	15 (79%)	4 (21%)	1	10
2	Z	15/23 (65%)	13 (87%)	2 (13%)	5	30
All	All	1022/1252 (82%)	965 (94%)	57 (6%)	26	67

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	85	ILE
1	A	103	ASP
1	A	120	THR
1	A	181	THR
1	A	246	SER
1	A	254	CYS
1	A	284	THR
1	A	296	TYR
1	A	315	ASP
1	B	71	VAL
1	B	80	SER
1	B	85	ILE
1	B	103	ASP
1	B	118	VAL
1	B	120	THR
1	B	160	ASP
1	B	246	SER
1	B	254	CYS
1	B	260	THR
1	B	284	THR
1	B	296	TYR
1	B	305	CYS
1	B	315	ASP
1	C	64	ASP
1	C	71	VAL
1	C	85	ILE
1	C	103	ASP
1	C	120	THR
1	C	212	ILE
1	C	246	SER
1	C	254	CYS
1	C	284	THR
1	C	305	CYS
1	D	71	VAL
1	D	85	ILE
1	D	103	ASP
1	D	120	THR
1	D	160	ASP
1	D	212	ILE
1	D	246	SER
1	D	254	CYS
1	D	280	ARG

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Mol	Chain	Res	Type
1	D	284	THR
2	E	594	LEU
2	E	598	GLN
2	E	600	SER
2	E	607	CYS
2	G	594	LEU
2	G	598	GLN
2	G	600	SER
2	G	607	CYS
2	Z	594	LEU
2	Z	607	CYS
2	F	594	LEU
2	F	600	SER
2	F	607	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	304	GLN
1	D	331	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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
3	GDP	A	401	-	23,30,30	1.15	2 (8%)	30,47,47	1.81	7 (23%)
4	CIT	A	402	-	3,12,12	1.33	0	3,17,17	2.68	2 (66%)
3	GDP	B	401	-	23,30,30	1.17	2 (8%)	30,47,47	1.78	7 (23%)
3	GDP	C	401	-	23,30,30	1.17	2 (8%)	30,47,47	1.87	7 (23%)
4	CIT	C	402	-	3,12,12	1.37	0	3,17,17	3.29	1 (33%)

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	GDP	A	401	-	-	0/12/32/32	0/3/3/3
4	CIT	A	402	-	-	0/6/16/16	0/0/0/0
3	GDP	B	401	-	-	0/12/32/32	0/3/3/3
3	GDP	C	401	-	-	0/12/32/32	0/3/3/3
4	CIT	C	402	-	-	0/6/16/16	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GDP	C5-C4	2.90	1.47	1.40
3	B	401	GDP	C5-C4	2.94	1.47	1.40
3	C	401	GDP	C5-C4	2.96	1.47	1.40
3	C	401	GDP	C6-C5	3.57	1.48	1.41
3	B	401	GDP	C6-C5	3.58	1.48	1.41
3	A	401	GDP	C6-C5	3.60	1.48	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	CIT	C3-C2-C1	-5.37	106.38	114.96
3	C	401	GDP	C5-C6-N1	-4.23	117.80	123.59
3	B	401	GDP	C5-C6-N1	-4.22	117.81	123.59
3	A	401	GDP	C5-C6-N1	-4.04	118.06	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	GDP	PA-O3A-PB	-3.83	119.82	132.67
4	A	402	CIT	C3-C4-C5	-3.72	109.02	114.96
3	C	401	GDP	PA-O3A-PB	-3.57	120.70	132.67
3	C	401	GDP	C2'-C1'-N9	-3.45	109.02	114.29
3	C	401	GDP	C4-C5-N7	-3.22	106.52	109.48
3	A	401	GDP	C6-C5-C4	-3.15	117.13	120.90
3	B	401	GDP	PA-O3A-PB	-3.14	122.12	132.67
3	A	401	GDP	C4-C5-N7	-3.14	106.59	109.48
3	B	401	GDP	C4-C5-N7	-3.11	106.62	109.48
3	C	401	GDP	N3-C2-N1	-3.04	122.81	127.44
3	A	401	GDP	N3-C2-N1	-3.04	122.81	127.44
3	C	401	GDP	C6-C5-C4	-2.95	117.38	120.90
3	B	401	GDP	N3-C2-N1	-2.93	122.98	127.44
3	B	401	GDP	C6-C5-C4	-2.87	117.47	120.90
4	A	402	CIT	C3-C2-C1	-2.77	110.53	114.96
3	B	401	GDP	C2'-C1'-N9	-2.49	110.48	114.29
3	A	401	GDP	C2'-C1'-N9	-2.08	111.11	114.29
3	A	401	GDP	C6-N1-C2	4.54	122.24	115.94
3	B	401	GDP	C6-N1-C2	4.55	122.25	115.94
3	C	401	GDP	C6-N1-C2	4.59	122.31	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GDP	4	0
4	A	402	CIT	1	0
3	B	401	GDP	6	0
3	C	401	GDP	2	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 ⓘ

### 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	317/330 (96%)	-0.33	1 (0%) 94 90	73, 128, 179, 209	0
1	B	316/330 (95%)	-0.34	2 (0%) 90 83	68, 122, 176, 208	0
1	C	311/330 (94%)	-0.30	0 100 100	64, 129, 182, 210	0
1	D	316/330 (95%)	-0.25	2 (0%) 90 83	72, 126, 180, 204	0
2	E	22/25 (88%)	-0.43	0 100 100	116, 145, 173, 213	0
2	F	22/25 (88%)	-0.18	0 100 100	93, 134, 170, 184	0
2	G	21/25 (84%)	-0.09	1 (4%) 34 23	123, 149, 172, 190	0
2	Z	19/25 (76%)	1.00	3 (15%) 3 3	144, 169, 213, 224	0
All	All	1344/1420 (94%)	-0.28	9 (0%) 89 81	64, 128, 181, 224	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	605	GLN	3.2
2	Z	603	ASP	2.8
2	Z	597	CYS	2.6
1	D	202	GLY	2.4
2	G	605	GLN	2.1
1	D	214	CYS	2.1
1	A	168	ILE	2.1
1	B	119	MET	2.1
1	B	114	ALA	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CIT	A	402	13/13	0.91	0.24	1.11	91,157,181,191	0
3	GDP	A	401	28/28	0.98	0.23	0.52	68,110,146,162	0
3	GDP	C	401	28/28	0.97	0.18	-0.27	73,111,173,186	0
4	CIT	C	402	13/13	0.92	0.21	-0.30	98,132,173,182	0
3	GDP	B	401	28/28	0.98	0.19	-0.61	47,110,144,189	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.