



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:57 AM GMT

PDB ID : 3QT2  
Title : Structure of a cytokine ligand-receptor complex  
Authors : Mueller, T.D.; Patino, E.; Kotzsch, A.; Saremba, S.; Nickel, J.; Schmitz, W.;  
Sebald, W.  
Deposited on : 2011-02-22  
Resolution : 2.55 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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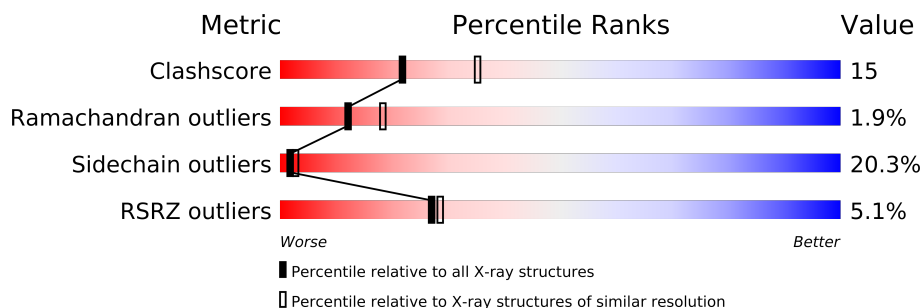
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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	317	
1	B	317	
2	C	117	
2	D	117	
2	E	117	
2	F	117	

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	BGC	A	316	-	X
3	BGC	A	317	-	X
3	BGC	A	318	-	X
3	BGC	B	316	-	X
3	BGC	B	317	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	BGC	B	318	-	X
4	MPD	A	319	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8581 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 Interleukin-5 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2463	1568	417	466	12			
1	B	307	Total	C	N	O	S	0	0	0
			2460	1565	416	467	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q01344
A	66	ALA	CYS	ENGINEERED MUTATION	UNP Q01344
A	72	MET	LYS	ENGINEERED MUTATION	UNP Q01344
A	138	MET	LEU	ENGINEERED MUTATION	UNP Q01344
A	167	MET	LYS	ENGINEERED MUTATION	UNP Q01344
A	234	MET	LEU	ENGINEERED MUTATION	UNP Q01344
A	313	PHE	ASN	SEE REMARK 999	UNP Q01344
A	314	SER	ASP	SEE REMARK 999	UNP Q01344
A	315	ARG	GLU	SEE REMARK 999	UNP Q01344
B	-1	MET	-	EXPRESSION TAG	UNP Q01344
B	66	ALA	CYS	ENGINEERED MUTATION	UNP Q01344
B	72	MET	LYS	ENGINEERED MUTATION	UNP Q01344
B	138	MET	LEU	ENGINEERED MUTATION	UNP Q01344
B	167	MET	LYS	ENGINEERED MUTATION	UNP Q01344
B	234	MET	LEU	ENGINEERED MUTATION	UNP Q01344
B	313	PHE	ASN	SEE REMARK 999	UNP Q01344
B	314	SER	ASP	SEE REMARK 999	UNP Q01344
B	315	ARG	GLU	SEE REMARK 999	UNP Q01344

- Molecule 2 is a protein called Interleukin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	110	Total	C	N	O	S	0	0	0
			886	563	155	165	3			

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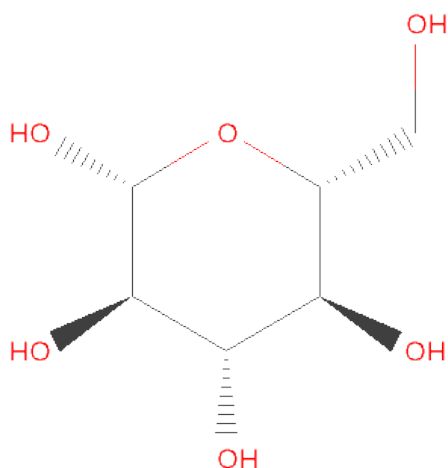
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	109	Total	C	N	O	S	0	0	0
			879	559	154	163	3			
2	E	109	Total	C	N	O	S	0	0	0
			879	559	154	163	3			
2	F	109	Total	C	N	O	S	0	0	0
			879	559	154	163	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	EXPRESSION TAG	UNP P05113
D	-1	MET	-	EXPRESSION TAG	UNP P05113
E	-1	MET	-	EXPRESSION TAG	UNP P05113
F	-1	MET	-	EXPRESSION TAG	UNP P05113

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



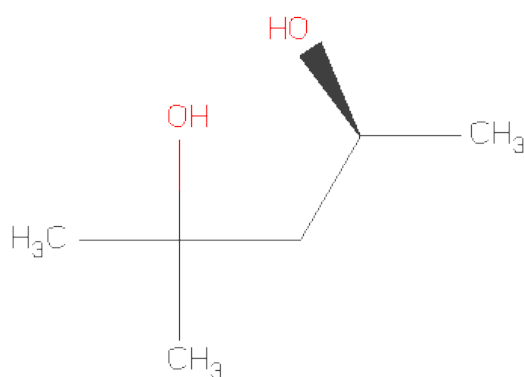
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

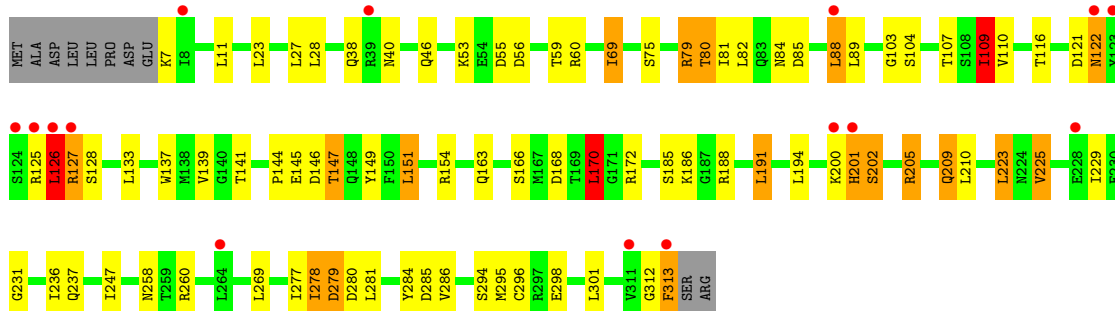
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	C	8	Total	O	0	0
			8	8		
5	D	9	Total	O	0	0
			9	9		
5	B	12	Total	O	0	0
			12	12		
5	E	7	Total	O	0	0
			7	7		
5	F	4	Total	O	0	0
			4	4		

### 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.

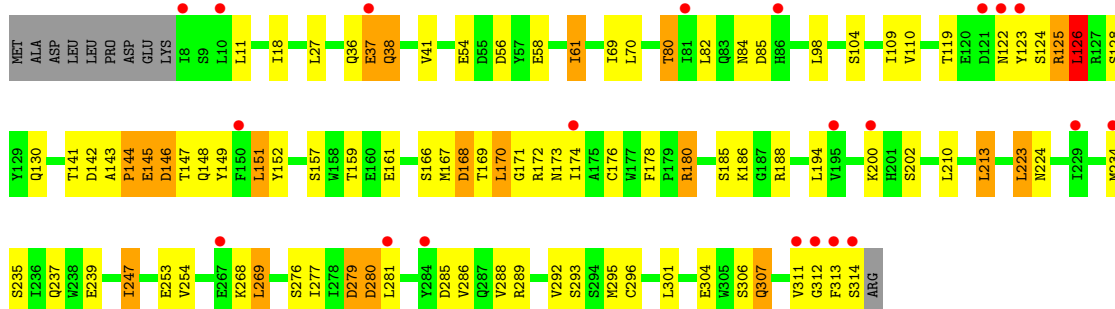
- Molecule 1: Interleukin-5 receptor subunit alpha

Chain A: 



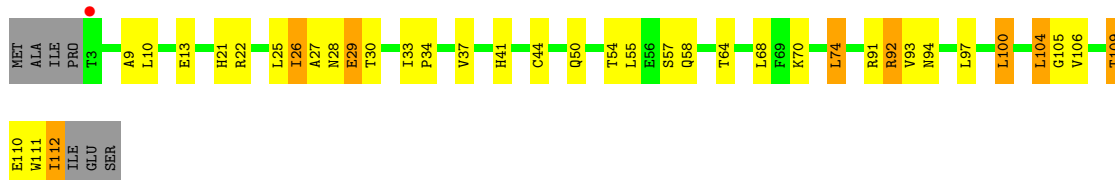
- Molecule 1: Interleukin-5 receptor subunit alpha

Chain B: 



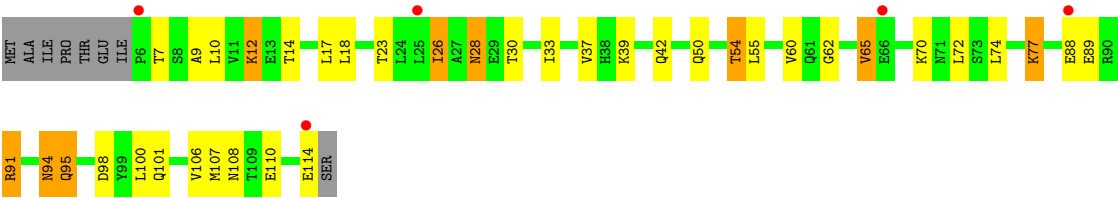
- Molecule 2: Interleukin-5

Chain C: 



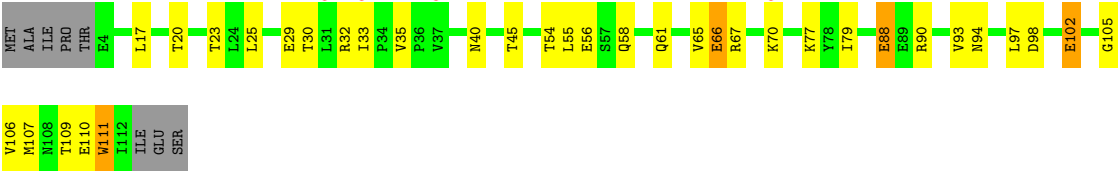
- Molecule 2: Interleukin-5

Chain D: 



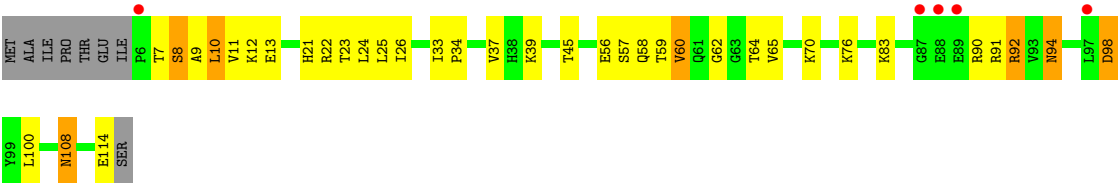
• Molecule 2: Interleukin-5

Chain E:



• Molecule 2: Interleukin-5

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.08Å 61.63Å 142.11Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	42.02 – 2.55 38.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.02-2.55) 99.8 (38.49-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.207 , 0.264 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	79.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36175 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% 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: MPD, BGC

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	0.97	6/2528 (0.2%)	0.82	2/3447 (0.1%)
1	B	0.94	10/2525 (0.4%)	0.81	5/3444 (0.1%)
2	C	0.86	0/899	0.77	0/1213
2	D	0.74	0/892	0.77	0/1202
2	E	0.91	1/892 (0.1%)	0.79	0/1203
2	F	0.77	0/892	0.75	1/1202 (0.1%)
All	All	0.90	17/8628 (0.2%)	0.80	8/11711 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLU	CD-OE2	14.60	1.41	1.25
1	A	145	GLU	CD-OE1	14.16	1.41	1.25
1	B	170	LEU	C-N	14.04	1.58	1.33
1	B	146	ASP	CG-OD1	10.78	1.50	1.25
1	A	145	GLU	CG-CD	8.07	1.64	1.51
1	A	170	LEU	C-O	7.98	1.38	1.23
1	B	170	LEU	C-O	7.15	1.36	1.23
1	B	146	ASP	CG-OD2	7.07	1.41	1.25
1	B	145	GLU	CG-CD	6.73	1.62	1.51
1	B	172	ARG	CZ-NH1	6.72	1.41	1.33
1	B	145	GLU	CD-OE1	6.56	1.32	1.25
1	A	172	ARG	CB-CG	5.96	1.68	1.52
2	E	102	GLU	CG-CD	5.94	1.60	1.51
1	B	172	ARG	CG-CD	5.51	1.65	1.51
1	B	168	ASP	CG-OD1	5.37	1.37	1.25
1	B	145	GLU	CB-CG	5.37	1.62	1.52
1	A	172	ARG	CZ-NH2	5.29	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	LEU	CA-CB-CG	9.37	136.85	115.30
1	B	146	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	B	172	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	151	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	213	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	191	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	126	LEU	CA-CB-CG	5.23	127.33	115.30
2	F	62	GLY	N-CA-C	-5.14	100.25	113.10

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	2463	0	193	38	0
1	B	2460	0	185	44	0
2	C	886	0	23	23	0
2	D	879	0	16	18	0
2	E	879	0	16	12	0
2	F	879	0	16	13	0
3	A	36	0	36	0	0
3	B	36	0	36	1	0
4	A	8	0	14	0	0
5	A	15	0	0	1	0
5	B	12	0	0	2	0
5	C	8	0	0	1	0
5	D	9	0	0	1	0
5	E	7	0	0	1	0
5	F	4	0	0	0	0
All	All	8581	0	535	137	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 15.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:123:TYR:CD2	1:B:180:ARG:NH2	1.85	1.44
1:B:123:TYR:HD2	1:B:180:ARG:NH2	0.92	1.41
1:B:295:MET:CE	2:F:12:LYS:CD	2.32	1.06
1:A:103:GLY:O	1:A:205:ARG:NH1	1.98	0.95
1:A:144:PRO:O	1:A:147:THR:CG2	2.20	0.89
1:A:46:GLN:OE1	1:A:79:ARG:NH1	2.07	0.88
3:B:317:BGC:H6C2	5:B:329:HOH:O	1.73	0.87
1:A:188:ARG:NH2	1:A:296:CYS:O	2.09	0.86
2:F:94:ASN:O	2:F:98:ASP:OD1	1.95	0.84
1:A:295:MET:SD	2:D:12:LYS:CG	2.66	0.83
2:D:26:ILE:O	2:D:26:ILE:CG1	2.27	0.82
1:B:188:ARG:NH2	1:B:296:CYS:O	2.13	0.81
1:B:234:MET:CE	1:B:311:VAL:CG1	2.60	0.80
1:A:201:HIS:O	1:A:202:SER:CB	2.32	0.78
1:A:205:ARG:NH1	1:A:205:ARG:CG	2.48	0.76
2:E:98:ASP:OD1	2:F:22:ARG:NH2	2.22	0.72
2:D:94:ASN:ND2	2:D:95:GLN:N	2.38	0.71
1:A:122:ASN:HA	1:A:127:ARG:HH22	1.54	0.70
1:B:36:GLN:O	1:B:38:GLN:HG3	1.92	0.70
2:C:111:TRP:CZ2	2:D:42:GLN:OE1	2.45	0.69
2:C:26:ILE:O	2:C:28:ASN:N	2.26	0.69
1:A:279:ASP:OD1	1:A:279:ASP:C	2.31	0.68
2:C:26:ILE:C	2:C:26:ILE:CD1	2.63	0.67
1:A:88:LEU:CD2	1:A:89:LEU:N	2.58	0.66
2:D:94:ASN:ND2	2:D:94:ASN:C	2.49	0.66
2:E:111:TRP:O	5:E:122:HOH:O	2.13	0.66
1:B:279:ASP:OD1	1:B:280:ASP:N	2.29	0.65
2:C:105:GLY:O	2:C:109:THR:CG2	2.45	0.65
1:A:122:ASN:N	1:A:122:ASN:OD1	2.30	0.64
1:B:130:GLN:NE2	1:B:180:ARG:NH1	2.46	0.64
1:B:295:MET:CE	2:F:12:LYS:CG	2.76	0.62
1:B:148:GLN:NE2	1:B:173:ASN:ND2	2.47	0.62
1:B:151:LEU:CD1	1:B:152:TYR:N	2.64	0.61
1:A:121:ASP:OD1	1:A:128:SER:O	2.19	0.61
2:E:40:ASN:ND2	2:E:111:TRP:CZ2	2.71	0.59
1:B:123:TYR:O	1:B:123:TYR:CG	2.56	0.59
2:C:111:TRP:O	2:C:112:ILE:CB	2.50	0.59
2:F:7:THR:O	2:F:8:SER:C	2.41	0.58
2:D:114:GLU:CG	2:D:114:GLU:O	2.51	0.58
1:B:84:ASN:OD1	1:B:85:ASP:N	2.37	0.58
1:B:279:ASP:C	1:B:279:ASP:OD1	2.42	0.58
2:F:92:ARG:NH1	2:F:92:ARG:CG	2.66	0.58
1:B:122:ASN:OD1	1:B:125:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:111:TRP:N	2:C:111:TRP:CD1	2.72	0.56
1:B:151:LEU:CD1	1:B:151:LEU:C	2.74	0.56
1:B:253:GLU:OE2	1:B:289:ARG:NH2	2.38	0.55
2:F:37:VAL:O	2:F:37:VAL:CG1	2.53	0.55
1:B:146:ASP:OD2	1:B:200:LYS:CD	2.55	0.55
2:C:100:LEU:CD2	2:C:104:LEU:CD2	2.85	0.55
1:A:312:GLY:C	1:A:313:PHE:CD1	2.80	0.55
2:D:114:GLU:HG3	2:D:114:GLU:O	2.07	0.55
1:B:58:GLU:OE2	2:E:90:ARG:NH1	2.40	0.54
1:A:23:LEU:O	1:A:154:ARG:NH1	2.41	0.54
2:C:100:LEU:CD2	2:C:100:LEU:O	2.56	0.54
1:B:168:ASP:O	1:B:170:LEU:N	2.42	0.53
1:A:278:ILE:CG1	1:A:284:TYR:CZ	2.91	0.53
1:B:288:VAL:N	1:B:306:SER:OG	2.42	0.53
1:B:280:ASP:OD1	1:B:280:ASP:N	2.41	0.53
2:D:62:GLY:O	2:D:65:VAL:CG1	2.56	0.53
1:B:126:LEU:H	1:B:126:LEU:CD1	2.20	0.53
2:E:35:VAL:CG1	2:F:91:ARG:CG	2.87	0.53
2:C:92:ARG:CG	5:C:116:HOH:O	2.56	0.52
1:A:258:ASN:OD1	1:A:260:ARG:N	2.43	0.52
2:C:93:VAL:O	2:C:94:ASN:C	2.47	0.52
1:A:59:THR:OG1	1:A:60:ARG:N	2.43	0.50
1:B:61:ILE:CD1	2:E:88:GLU:OE1	2.59	0.50
1:A:84:ASN:C	1:A:84:ASN:OD1	2.49	0.50
2:E:93:VAL:O	2:E:94:ASN:C	2.48	0.49
2:C:41:HIS:O	2:C:44:CYS:N	2.45	0.49
1:B:224:ASN:ND2	1:B:239:GLU:OE2	2.45	0.49
2:F:21:HIS:CE1	2:F:64:THR:OG1	2.65	0.49
1:A:209:GLN:NE2	5:A:329:HOH:O	2.46	0.48
2:C:74:LEU:CD2	2:C:74:LEU:C	2.82	0.48
2:C:100:LEU:CD2	2:C:100:LEU:C	2.80	0.48
2:E:35:VAL:CG1	2:E:35:VAL:O	2.62	0.48
2:D:89:GLU:OE2	2:D:91:ARG:NH2	2.47	0.48
1:B:145:GLU:N	5:B:328:HOH:O	2.46	0.48
2:C:29:GLU:OE1	2:C:29:GLU:CA	2.62	0.48
1:A:280:ASP:OD1	1:A:280:ASP:N	2.45	0.48
1:B:123:TYR:CD2	1:B:123:TYR:O	2.67	0.47
1:A:125:ARG:O	1:A:126:LEU:HB2	2.15	0.47
2:C:10:LEU:CD2	2:C:10:LEU:C	2.83	0.47
1:A:69:ILE:CD1	1:A:209:GLN:CA	2.93	0.47
2:C:21:HIS:O	2:C:22:ARG:C	2.53	0.46
1:B:130:GLN:CD	1:B:180:ARG:NH1	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:9:ALA:O	2:F:10:LEU:C	2.53	0.46
2:C:9:ALA:O	2:C:13:GLU:N	2.49	0.46
1:B:312:GLY:C	1:B:313:PHE:CD1	2.89	0.46
2:E:105:GLY:O	2:E:109:THR:OG1	2.34	0.46
2:C:26:ILE:CD1	2:C:26:ILE:O	2.64	0.45
1:B:279:ASP:OD1	1:B:281:LEU:N	2.49	0.45
1:B:125:ARG:HD3	1:B:125:ARG:HA	1.54	0.45
2:C:33:ILE:O	2:C:34:PRO:C	2.54	0.45
2:E:111:TRP:N	2:E:111:TRP:CD1	2.84	0.45
1:B:168:ASP:O	1:B:171:GLY:N	2.50	0.44
2:F:33:ILE:CG2	2:F:34:PRO:N	2.80	0.44
2:C:33:ILE:N	2:D:91:ARG:O	2.50	0.44
2:F:56:GLU:O	2:F:58:GLN:N	2.51	0.44
1:B:147:THR:CG2	1:B:148:GLN:N	2.80	0.44
1:A:313:PHE:N	1:A:313:PHE:CD1	2.82	0.44
1:A:56:ASP:OD1	1:A:56:ASP:N	2.50	0.44
1:B:306:SER:O	1:B:307:GLN:C	2.55	0.44
1:A:146:ASP:OD2	1:A:200:LYS:N	2.51	0.43
1:A:139:VAL:O	1:A:149:TYR:OH	2.36	0.43
1:A:168:ASP:OD1	1:A:170:LEU:N	2.52	0.43
2:E:40:ASN:OD1	2:E:40:ASN:C	2.57	0.43
1:B:223:LEU:CD1	1:B:223:LEU:N	2.81	0.43
2:C:22:ARG:NH1	2:D:98:ASP:OD1	2.51	0.43
1:B:148:GLN:NE2	1:B:173:ASN:CG	2.72	0.43
1:A:258:ASN:OD1	1:A:258:ASN:C	2.56	0.43
1:A:121:ASP:CG	1:A:121:ASP:O	2.57	0.42
2:D:7:THR:OG1	2:D:7:THR:O	2.34	0.42
2:D:9:ALA:CA	5:D:123:HOH:O	2.67	0.42
1:B:152:TYR:CE2	1:B:161:GLU:CG	3.02	0.42
1:B:269:LEU:CD2	1:B:269:LEU:N	2.81	0.42
1:A:104:SER:O	1:A:107:THR:OG1	2.37	0.42
2:D:37:VAL:CG2	2:D:37:VAL:O	2.67	0.42
1:A:121:ASP:O	1:A:127:ARG:NH1	2.52	0.42
1:A:55:ASP:OD2	2:C:91:ARG:NH2	2.53	0.42
2:C:110:GLU:C	2:C:111:TRP:CD1	2.93	0.41
1:B:109:ILE:CG2	1:B:149:TYR:CE1	3.03	0.41
2:D:28:ASN:ND2	2:D:30:THR:OG1	2.53	0.41
1:B:38:GLN:H	1:B:38:GLN:HG3	1.58	0.41
1:B:166:SER:O	1:B:174:ILE:N	2.54	0.41
1:B:176:CYS:SG	1:B:178:PHE:CE2	3.14	0.41
1:A:109:ILE:CG1	1:A:137:TRP:CD1	3.04	0.41
2:D:50:GLN:O	2:D:54:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:ARG:HD2	1:A:127:ARG:HA	1.42	0.41
1:A:11:LEU:O	1:A:80:THR:CG2	2.69	0.41
1:A:109:ILE:CD1	1:A:137:TRP:CD1	3.04	0.40
1:A:223:LEU:N	1:A:223:LEU:HD12	2.36	0.40
1:B:11:LEU:O	1:B:80:THR:CG2	2.70	0.40
1:B:143:ALA:O	1:B:144:PRO:C	2.60	0.40
2:E:35:VAL:CG1	2:F:91:ARG:CD	2.99	0.40
2:D:74:LEU:O	2:D:77:LYS:N	2.54	0.40
1:A:225:VAL:HA	1:A:237:GLN:O	2.21	0.40
2:D:106:VAL:C	2:D:108:ASN:N	2.74	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	305/317 (96%)	279 (92%)	20 (7%)	6 (2%)	11	17
1	B	305/317 (96%)	281 (92%)	17 (6%)	7 (2%)	10	13
2	C	108/117 (92%)	97 (90%)	10 (9%)	1 (1%)	25	41
2	D	107/117 (92%)	96 (90%)	10 (9%)	1 (1%)	25	41
2	E	107/117 (92%)	103 (96%)	3 (3%)	1 (1%)	25	41
2	F	107/117 (92%)	99 (92%)	4 (4%)	4 (4%)	5	6
All	All	1039/1102 (94%)	955 (92%)	64 (6%)	20 (2%)	12	18

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	202	SER
2	C	27	ALA
1	B	169	THR
2	E	66	GLU

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Mol	Chain	Res	Type
2	F	60	VAL
1	A	186	LYS
1	B	124	SER
1	B	186	LYS
1	B	247	ILE
2	F	57	SER
2	D	10	LEU
1	B	37	GLU
1	B	144	PRO
2	F	108	ASN
1	A	85	ASP
1	B	304	GLU
2	F	8	SER
1	A	231	GLY
1	A	109	ILE

### 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	274/283 (97%)	225 (82%)	49 (18%)	2	4
1	B	274/283 (97%)	225 (82%)	49 (18%)	2	4
2	C	100/106 (94%)	79 (79%)	21 (21%)	1	2
2	D	99/106 (93%)	75 (76%)	24 (24%)	1	1
2	E	99/106 (93%)	72 (73%)	27 (27%)	0	0
2	F	99/106 (93%)	77 (78%)	22 (22%)	1	2
All	All	945/990 (96%)	753 (80%)	192 (20%)	2	3

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	27	LEU
1	A	28	LEU
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	40	ASN
1	A	53	LYS
1	A	69	ILE
1	A	75	SER
1	A	79	ARG
1	A	80	THR
1	A	81	ILE
1	A	82	LEU
1	A	88	LEU
1	A	109	ILE
1	A	110	VAL
1	A	116	THR
1	A	122	ASN
1	A	126	LEU
1	A	127	ARG
1	A	133	LEU
1	A	141	THR
1	A	147	THR
1	A	151	LEU
1	A	163	GLN
1	A	166	SER
1	A	170	LEU
1	A	185	SER
1	A	191	LEU
1	A	194	LEU
1	A	201	HIS
1	A	205	ARG
1	A	209	GLN
1	A	210	LEU
1	A	223	LEU
1	A	225	VAL
1	A	229	ILE
1	A	236	ILE
1	A	247	ILE
1	A	269	LEU
1	A	277	ILE
1	A	278	ILE
1	A	279	ASP
1	A	281	LEU
1	A	285	ASP
1	A	286	VAL
1	A	294	SER

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Mol	Chain	Res	Type
1	A	298	GLU
1	A	301	LEU
1	A	313	PHE
2	C	25	LEU
2	C	26	ILE
2	C	29	GLU
2	C	30	THR
2	C	37	VAL
2	C	50	GLN
2	C	54	THR
2	C	55	LEU
2	C	57	SER
2	C	58	GLN
2	C	64	THR
2	C	68	LEU
2	C	70	LYS
2	C	74	LEU
2	C	92	ARG
2	C	97	LEU
2	C	100	LEU
2	C	104	LEU
2	C	106	VAL
2	C	109	THR
2	C	112	ILE
2	D	12	LYS
2	D	14	THR
2	D	17	LEU
2	D	18	LEU
2	D	23	THR
2	D	26	ILE
2	D	28	ASN
2	D	33	ILE
2	D	39	LYS
2	D	54	THR
2	D	55	LEU
2	D	60	VAL
2	D	65	VAL
2	D	70	LYS
2	D	72	LEU
2	D	77	LYS
2	D	88	GLU
2	D	91	ARG

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Mol	Chain	Res	Type
2	D	94	ASN
2	D	95	GLN
2	D	100	LEU
2	D	101	GLN
2	D	107	MET
2	D	110	GLU
1	B	18	ILE
1	B	27	LEU
1	B	37	GLU
1	B	38	GLN
1	B	41	VAL
1	B	54	GLU
1	B	56	ASP
1	B	61	ILE
1	B	69	ILE
1	B	70	LEU
1	B	80	THR
1	B	82	LEU
1	B	98	LEU
1	B	104	SER
1	B	110	VAL
1	B	119	THR
1	B	125	ARG
1	B	126	LEU
1	B	128	SER
1	B	141	THR
1	B	142	ASP
1	B	151	LEU
1	B	157	SER
1	B	159	THR
1	B	167	MET
1	B	180	ARG
1	B	185	SER
1	B	194	LEU
1	B	202	SER
1	B	210	LEU
1	B	213	LEU
1	B	223	LEU
1	B	235	SER
1	B	237	GLN
1	B	247	ILE
1	B	254	VAL

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Mol	Chain	Res	Type
1	B	268	LYS
1	B	269	LEU
1	B	276	SER
1	B	277	ILE
1	B	279	ASP
1	B	280	ASP
1	B	285	ASP
1	B	286	VAL
1	B	292	VAL
1	B	293	SER
1	B	301	LEU
1	B	307	GLN
1	B	314	SER
2	E	17	LEU
2	E	20	THR
2	E	23	THR
2	E	25	LEU
2	E	29	GLU
2	E	30	THR
2	E	32	ARG
2	E	33	ILE
2	E	45	THR
2	E	54	THR
2	E	55	LEU
2	E	56	GLU
2	E	58	GLN
2	E	61	GLN
2	E	65	VAL
2	E	66	GLU
2	E	67	ARG
2	E	70	LYS
2	E	77	LYS
2	E	79	ILE
2	E	88	GLU
2	E	97	LEU
2	E	102	GLU
2	E	106	VAL
2	E	107	MET
2	E	110	GLU
2	E	111	TRP
2	F	10	LEU
2	F	11	VAL

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Mol	Chain	Res	Type
2	F	13	GLU
2	F	23	THR
2	F	24	LEU
2	F	25	LEU
2	F	26	ILE
2	F	39	LYS
2	F	45	THR
2	F	59	THR
2	F	60	VAL
2	F	65	VAL
2	F	70	LYS
2	F	76	LYS
2	F	83	LYS
2	F	90	ARG
2	F	92	ARG
2	F	94	ASN
2	F	98	ASP
2	F	100	LEU
2	F	108	ASN
2	F	114	GLU

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

Mol	Chain	Res	Type
1	B	40	ASN
1	B	86	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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	BGC	A	316	-	12,12,12	0.49	0	17,17,17	1.02	1 (5%)
3	BGC	A	317	-	12,12,12	0.60	0	17,17,17	1.47	3 (17%)
3	BGC	A	318	-	12,12,12	0.51	0	17,17,17	1.02	1 (5%)
4	MPD	A	319	-	7,7,7	0.42	0	10,10,10	0.26	0
3	BGC	B	316	-	12,12,12	0.46	0	17,17,17	0.60	0
3	BGC	B	317	-	12,12,12	0.58	0	17,17,17	1.25	3 (17%)
3	BGC	B	318	-	12,12,12	0.51	0	17,17,17	0.72	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	BGC	A	316	-	-	0/2/22/22	0/1/1/1
3	BGC	A	317	-	-	0/2/22/22	0/1/1/1
3	BGC	A	318	-	-	0/2/22/22	0/1/1/1
4	MPD	A	319	-	-	0/5/5/5	0/0/0/0
3	BGC	B	316	-	-	0/2/22/22	0/1/1/1
3	BGC	B	317	-	-	0/2/22/22	0/1/1/1
3	BGC	B	318	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	317	BGC	O5-C1-C2	3.87	115.85	109.86
3	A	317	BGC	C1-C2-C3	2.92	115.17	110.53
3	B	317	BGC	C1-C2-C3	-2.81	106.09	110.53
3	A	317	BGC	C1-O5-C5	2.64	118.12	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	316	BGC	O5-C5-C6	2.41	112.26	106.34
3	A	318	BGC	O5-C1-C2	2.29	113.42	109.86
3	B	317	BGC	C3-C4-C5	2.23	114.18	110.20
3	B	317	BGC	O5-C5-C4	2.11	113.66	109.76

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	307/317 (96%)	0.60	15 (4%)	28 30	49, 74, 120, 142	0
1	B	307/317 (96%)	0.60	21 (6%)	17 17	49, 74, 122, 153	0
2	C	110/117 (94%)	0.43	1 (0%)	81 83	51, 74, 116, 123	0
2	D	109/117 (93%)	0.55	5 (4%)	31 33	52, 86, 117, 142	0
2	E	109/117 (93%)	0.35	4 (3%)	39 42	52, 73, 103, 122	0
2	F	109/117 (93%)	0.47	5 (4%)	31 33	54, 80, 115, 135	0
All	All	1051/1102 (95%)	0.54	51 (4%)	27 30	49, 76, 118, 153	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	TYR	6.1
1	B	313	PHE	4.9
1	A	122	ASN	4.8
1	B	123	TYR	4.4
1	A	125	ARG	4.3
1	A	200	LYS	4.3
1	A	126	LEU	4.2
1	A	201	HIS	4.2
2	D	88	GLU	4.0
2	F	6	PRO	3.8
2	D	6	PRO	3.6
1	A	127	ARG	3.6
2	E	37	VAL	3.5
1	B	314	SER	3.3
1	B	8	ILE	3.3
2	F	88	GLU	3.3
2	F	87	GLY	3.2
1	B	311	VAL	3.2
1	B	86	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	264	LEU	2.9
2	F	97	LEU	2.9
1	B	195	VAL	2.9
2	E	33	ILE	2.9
1	A	39	ARG	2.8
1	B	229	ILE	2.8
1	B	122	ASN	2.8
1	A	88	LEU	2.7
1	A	124	SER	2.7
2	C	3	THR	2.7
1	B	312	GLY	2.6
1	B	234	MET	2.6
1	A	311	VAL	2.5
1	A	313	PHE	2.5
1	B	37	GLU	2.4
1	B	284	TYR	2.4
2	D	114	GLU	2.4
2	F	89	GLU	2.4
1	B	281	LEU	2.3
1	B	121	ASP	2.2
2	D	66	GLU	2.2
2	E	70	LYS	2.2
1	B	200	LYS	2.2
1	A	8	ILE	2.2
2	E	31	LEU	2.2
1	B	10	LEU	2.1
2	D	25	LEU	2.1
1	A	228	GLU	2.1
1	B	267	GLU	2.1
1	B	81	ILE	2.1
1	B	174	ILE	2.0
1	B	150	PHE	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
3	BGC	B	316	12/12	0.23	8.67	115,119,120,122	0
3	BGC	A	318	12/12	0.36	8.51	128,132,134,134	0
3	BGC	A	317	12/12	0.39	5.76	117,121,122,122	0
3	BGC	B	317	12/12	0.42	4.32	139,140,142,143	0
4	MPD	A	319	8/8	0.36	4.14	104,107,110,111	0
3	BGC	B	318	12/12	0.32	3.97	129,132,133,134	0
3	BGC	A	316	12/12	0.22	2.02	118,121,122,123	0

## 6.5 Other polymers

There are no such residues in this entry.