



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:34 PM GMT

PDB ID : 4P9X  
Title : Structure of ConA/Rh3Glu complex  
Authors : Sakai, F.; Weiss, M.S.; Chen, G.  
Deposited on : 2014-04-06  
Resolution : 2.06 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

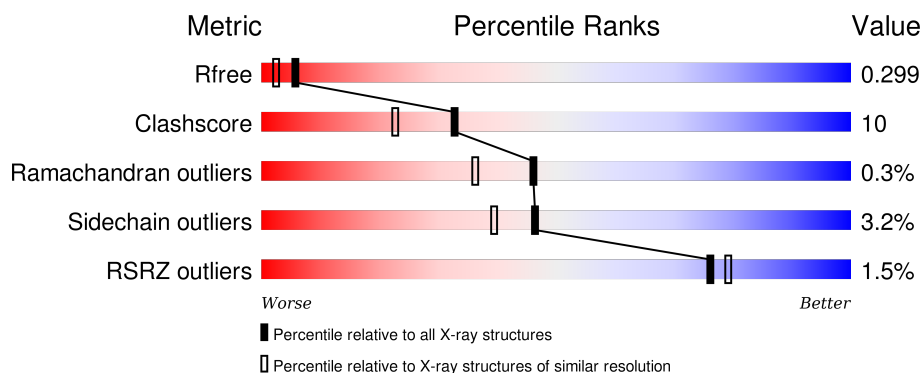
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	237	<div> <div>2%</div> <div>78% 19% ..</div> </div>
1	B	237	<div> <div>2%</div> <div>76% 22% .</div> </div>
1	C	237	<div> <div>2%</div> <div>79% 20% .</div> </div>
1	D	237	<div> <div>2%</div> <div>79% 19% .</div> </div>

## 2 Entry composition [i](#)

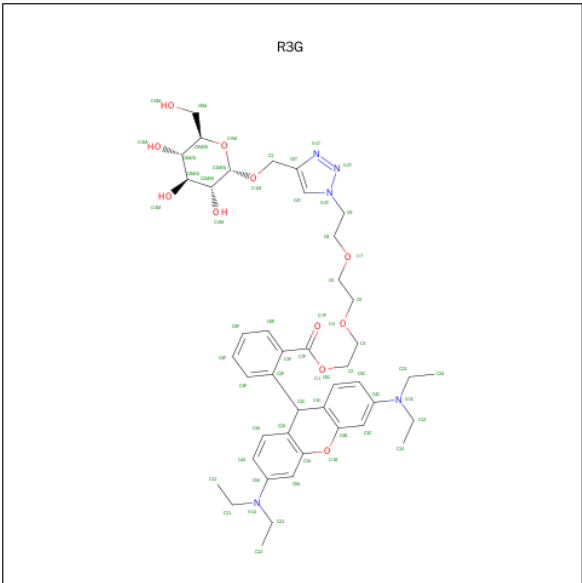
There are 5 unique types of molecules in this entry. The entry contains 7594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Concanavalin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	B	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	C	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	D	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

- Molecule 2 is 2-[2-(2-{4-[(alpha-D-glucopyranosyloxy)methyl]-1H-1,2,3-triazol-1-yl}ethoxy)ethoxy]ethyl 2-[3,6-bis(diethylamino)-9H-xanthen-9-yl]benzoate (three-letter code: R3G) (formula: C<sub>43</sub>H<sub>57</sub>N<sub>5</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			59	43	5	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			59	43	5	11		
2	C	1	Total	C	N	O	0	0
			59	43	5	11		
2	D	1	Total	C	N	O	0	0
			59	43	5	11		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

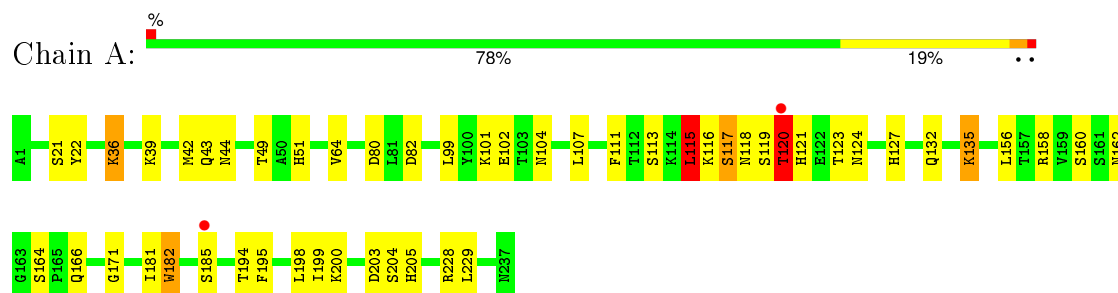
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	23	Total	O	0	0
			23	23		
5	C	39	Total	O	0	0
			39	39		
5	D	22	Total	O	0	0
			22	22		

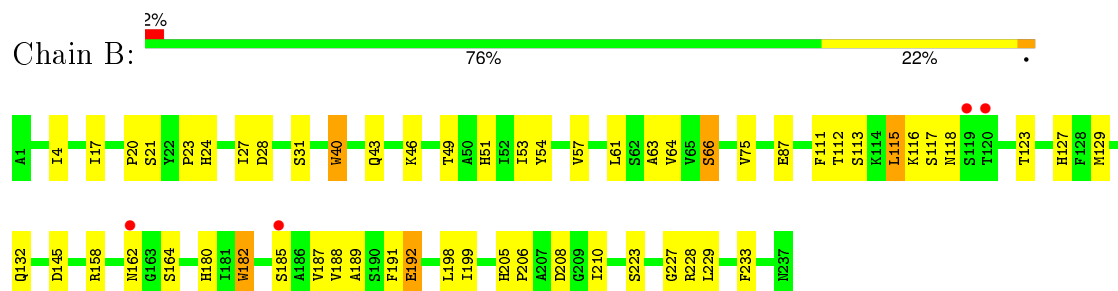
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

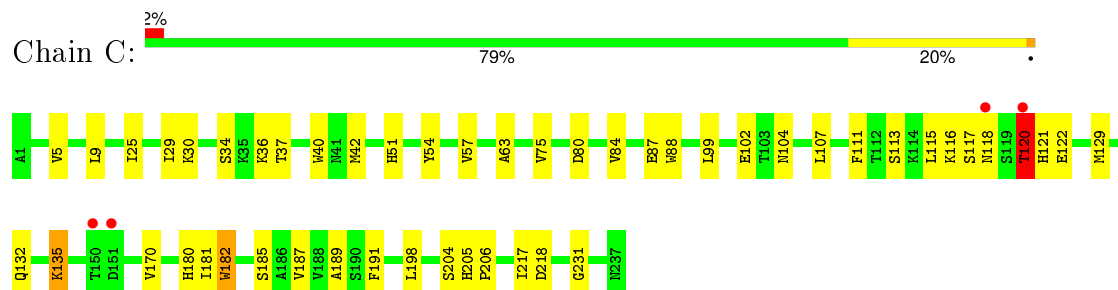
#### • Molecule 1: Concanavalin-A



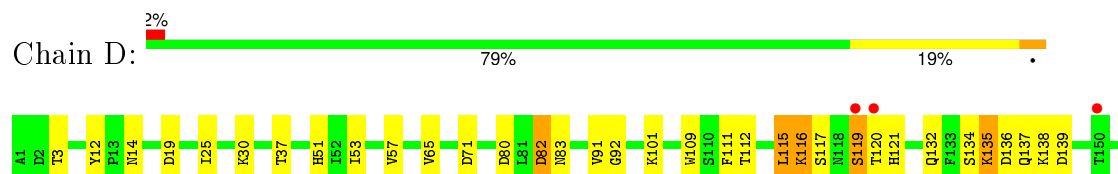
#### • Molecule 1: Concanavalin-A

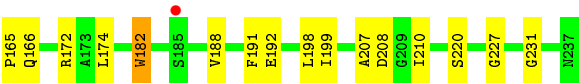


#### • Molecule 1: Concanavalin-A



#### • Molecule 1: Concanavalin-A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.17Å 116.03Å 84.25Å 90.00° 95.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.06 39.41 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.06) 99.4 (39.41-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.245 , 0.295 0.248 , 0.299	Depositor DCC
$R_{free}$ test set	2980 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.409 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	1 of 98988 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, R3G, MN

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	1.03	1/1851 (0.1%)	1.03	2/2522 (0.1%)
1	B	0.93	2/1851 (0.1%)	0.98	1/2522 (0.0%)
1	C	1.03	2/1851 (0.1%)	0.98	1/2522 (0.0%)
1	D	0.95	1/1851 (0.1%)	0.99	2/2522 (0.1%)
All	All	0.99	6/7404 (0.1%)	0.99	6/10088 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	TRP	CD2-CE2	6.76	1.49	1.41
1	D	182	TRP	CD2-CE2	5.99	1.48	1.41
1	A	182	TRP	CD2-CE2	5.36	1.47	1.41
1	B	182	TRP	CD2-CE2	5.35	1.47	1.41
1	B	40	TRP	CD2-CE2	5.29	1.47	1.41
1	C	182	TRP	CD2-CE2	5.07	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	MET	CG-SD-CE	-7.40	88.35	100.20
1	D	71	ASP	CB-CG-OD1	6.79	124.41	118.30
1	D	115	LEU	CA-CB-CG	6.36	129.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	228	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	129	MET	CG-SD-CE	-6.07	90.48	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	119	SER	Peptide

## 5.2 Too-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 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	1809	0	1755	44	0
1	B	1809	0	1755	36	0
1	C	1809	0	1755	40	0
1	D	1809	0	1755	42	0
2	A	59	0	56	2	0
2	B	59	0	56	1	0
2	C	59	0	56	5	0
2	D	59	0	56	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	30	0	0	2	0
5	B	23	0	0	2	0
5	C	39	0	0	1	0
5	D	22	0	0	2	0
All	All	7594	0	7244	153	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 10.

All (153) 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:B:66:SER:HB2	5:B:423:HOH:O	1.37	1.21
1:D:135:LYS:H	1:D:135:LYS:HD3	1.10	1.11
1:A:135:LYS:N	1:A:135:LYS:HD3	1.73	1.03
1:D:135:LYS:CD	1:D:135:LYS:H	1.80	0.94
1:A:135:LYS:H	1:A:135:LYS:HD3	1.32	0.94
1:A:135:LYS:H	1:A:135:LYS:CD	1.83	0.91
1:A:36:LYS:HE2	5:A:420:HOH:O	1.72	0.89
2:C:301:R3G:H30	2:C:301:R3G:H28	1.61	0.81
1:B:49:THR:OG1	1:D:121:HIS:HD2	1.65	0.80
1:D:135:LYS:N	1:D:135:LYS:HD3	1.94	0.79
1:B:57:VAL:HG23	1:B:188:VAL:HG23	1.67	0.77
1:C:115:LEU:HD23	1:C:189:ALA:HB2	1.65	0.76
1:A:120:THR:HG23	1:A:120:THR:O	1.84	0.75
1:A:42:MET:HE3	1:A:199:ILE:HB	1.69	0.74
1:A:160:SER:HB3	1:A:166:GLN:HE21	1.52	0.74
1:B:17:ILE:HD13	1:B:228:ARG:HD3	1.74	0.69
1:B:49:THR:OG1	1:D:121:HIS:CD2	2.46	0.69
1:B:145:ASP:OD1	1:B:158:ARG:NH2	2.27	0.67
1:A:120:THR:O	1:A:120:THR:CG2	2.42	0.67
1:C:30:LYS:HD2	1:C:84:VAL:HG13	1.76	0.67
1:A:39:LYS:NZ	5:A:425:HOH:O	2.28	0.66
1:D:80:ASP:OD2	5:D:408:HOH:O	2.13	0.66
1:D:3:THR:HG23	1:D:30:LYS:HD3	1.78	0.66
1:C:118:ASN:N	1:C:185:SER:O	2.25	0.66
1:C:122:GLU:HB2	1:D:132:GLN:HG3	1.78	0.65
1:C:80:ASP:OD2	5:C:415:HOH:O	2.15	0.65
1:B:28:ASP:HB3	1:B:31:SER:O	1.98	0.64
1:D:136:ASP:OD2	1:D:138:LYS:HE2	1.98	0.63
1:C:117:SER:O	1:C:121:HIS:HA	1.98	0.63
1:A:64:VAL:HG21	1:C:57:VAL:CG2	2.29	0.62
1:D:12:TYR:CD1	2:D:301:R3G:H57	2.34	0.62
1:A:135:LYS:H	1:A:135:LYS:CE	2.12	0.62
1:A:49:THR:OG1	1:C:121:HIS:HD2	1.83	0.62
1:B:180:HIS:CD2	1:B:182:TRP:O	2.53	0.61
1:A:111:PHE:CE2	1:A:113:SER:HB2	2.35	0.61
1:C:116:LYS:HB2	1:C:187:VAL:HG22	1.82	0.61
1:C:181:ILE:HD12	1:C:182:TRP:CD1	2.36	0.61
1:C:115:LEU:CD2	1:C:189:ALA:HB2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HG3	1:A:123:THR:OG1	2.02	0.60
1:B:53:ILE:HG22	1:B:192:GLU:HB3	1.83	0.60
1:D:116:LYS:N	1:D:116:LYS:HE3	2.16	0.59
1:D:82:ASP:HB3	1:D:182:TRP:CD2	2.37	0.59
1:A:118:ASN:N	1:A:185:SER:O	2.30	0.59
1:C:102:GLU:OE2	1:C:104:ASN:ND2	2.30	0.59
2:C:301:R3G:H28	2:C:301:R3G:C5C	2.33	0.58
1:D:199:ILE:HD11	1:D:210:ILE:HD12	1.84	0.58
1:B:116:LYS:HE2	1:D:51:HIS:HE1	1.68	0.58
1:D:101:LYS:HD2	1:D:165:PRO:O	2.04	0.57
1:C:204:SER:OG	1:C:205:HIS:HD2	1.88	0.57
1:A:101:LYS:NZ	1:A:203:ASP:OD1	2.38	0.56
1:C:116:LYS:HB2	1:C:187:VAL:CG2	2.36	0.56
1:A:51:HIS:CE1	1:C:116:LYS:HD2	2.40	0.56
1:D:117:SER:OG	1:D:119:SER:O	2.23	0.56
1:D:82:ASP:HB3	1:D:182:TRP:CG	2.41	0.56
1:B:111:PHE:CE2	1:B:113:SER:HB2	2.41	0.56
1:D:57:VAL:HG23	1:D:188:VAL:HG23	1.88	0.55
1:D:91:VAL:HG11	1:D:111:PHE:CE1	2.42	0.54
1:B:116:LYS:HB3	1:B:187:VAL:HG22	1.89	0.54
1:B:51:HIS:O	1:B:63:ALA:HA	2.07	0.53
1:A:156:LEU:O	1:A:171:GLY:HA3	2.08	0.53
1:A:49:THR:OG1	1:C:121:HIS:CD2	2.62	0.53
1:A:102:GLU:OE2	1:A:104:ASN:ND2	2.37	0.53
1:B:116:LYS:HE2	1:D:51:HIS:CE1	2.44	0.53
1:D:25:ILE:HG21	1:D:65:VAL:HG21	1.91	0.52
1:B:208:ASP:OD2	1:B:227:GLY:HA2	2.09	0.52
1:D:12:TYR:CE1	2:D:301:R3G:H57	2.45	0.52
1:B:64:VAL:HG21	1:D:57:VAL:HG22	1.92	0.52
1:B:87:GLU:HG3	1:B:182:TRP:O	2.09	0.52
1:D:208:ASP:OD2	1:D:227:GLY:HA2	2.10	0.52
1:C:217:ILE:HG13	1:C:218:ASP:N	2.24	0.51
1:D:14:ASN:O	1:D:19:ASP:HB2	2.09	0.51
1:B:20:PRO:HD2	1:B:24:HIS:CE1	2.46	0.51
1:A:107:LEU:HD12	1:A:107:LEU:N	2.26	0.51
1:D:82:ASP:HA	1:D:182:TRP:CD1	2.46	0.50
1:A:64:VAL:HG21	1:C:57:VAL:HG22	1.93	0.50
1:D:80:ASP:O	1:D:83:ASN:HB2	2.11	0.50
1:D:220:SER:HB2	5:D:410:HOH:O	2.13	0.49
1:A:64:VAL:HG21	1:C:57:VAL:HG21	1.94	0.49
1:B:23:PRO:HB2	1:B:40:TRP:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:SER:HB2	1:D:135:LYS:NZ	2.27	0.49
1:A:160:SER:HB3	1:A:166:GLN:NE2	2.26	0.49
1:B:17:ILE:CD1	1:B:228:ARG:HD3	2.41	0.49
1:A:162:ASN:OD1	1:A:164:SER:HB2	2.12	0.48
1:B:199:ILE:HD11	1:B:210:ILE:HD12	1.95	0.48
1:C:181:ILE:HD12	1:C:182:TRP:HD1	1.76	0.48
1:C:51:HIS:O	1:C:63:ALA:HA	2.14	0.48
1:A:80:ASP:OD1	1:A:82:ASP:HB2	2.14	0.47
1:A:64:VAL:CG2	1:C:57:VAL:HG21	2.45	0.47
1:C:88:TRP:HH2	1:D:137:GLN:NE2	2.13	0.46
2:B:301:R3G:H26	2:B:301:R3G:H30	1.64	0.46
1:C:115:LEU:HD23	1:C:189:ALA:CB	2.41	0.46
1:A:99:LEU:HD12	2:A:301:R3G:H49	1.98	0.46
1:B:4:ILE:HB	1:B:233:PHE:CE1	2.51	0.46
1:A:204:SER:OG	1:A:205:HIS:HD2	1.98	0.46
1:D:115:LEU:C	1:D:116:LYS:HE3	2.37	0.46
1:A:135:LYS:H	1:A:135:LYS:HE2	1.80	0.45
1:A:127:HIS:HB3	1:B:127:HIS:HB3	1.98	0.45
1:B:115:LEU:O	1:B:123:THR:HA	2.15	0.45
1:C:5:VAL:HG13	1:C:29:ILE:HD13	1.97	0.45
1:B:66:SER:CB	5:B:423:HOH:O	2.19	0.45
2:D:301:R3G:C2C	2:D:301:R3G:O1	2.65	0.45
1:A:115:LEU:HD12	1:A:124:ASN:HB2	1.98	0.45
1:D:120:THR:O	1:D:120:THR:HG23	2.16	0.45
1:A:64:VAL:CG2	1:C:57:VAL:CG2	2.95	0.45
1:B:115:LEU:HD22	1:B:189:ALA:HB1	1.99	0.44
1:B:27:ILE:HD12	1:B:75:VAL:HG13	1.99	0.44
1:A:44:ASN:OD1	1:A:200:LYS:HA	2.18	0.44
1:A:158:ARG:HG2	1:A:166:GLN:OE1	2.18	0.44
1:D:3:THR:HG23	1:D:30:LYS:CD	2.46	0.44
1:D:139:ASP:N	1:D:139:ASP:OD1	2.50	0.44
1:B:115:LEU:HD22	1:B:189:ALA:CB	2.47	0.43
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.80	0.43
1:A:42:MET:HE2	1:A:43:GLN:C	2.38	0.43
1:C:5:VAL:HG13	1:C:29:ILE:CD1	2.49	0.43
1:B:54:TYR:HB2	1:B:61:LEU:HD12	2.01	0.43
1:B:43:GLN:HE22	1:B:46:LYS:NZ	2.16	0.43
1:C:99:LEU:HD22	2:C:301:R3G:H11	2.00	0.43
2:D:301:R3G:H14	2:D:301:R3G:H18	1.76	0.43
1:A:117:SER:O	1:A:121:HIS:HA	2.19	0.42
1:C:25:ILE:HD12	1:C:75:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:HG22	1:A:195:PHE:N	2.34	0.42
1:B:118:ASN:N	1:B:185:SER:O	2.41	0.42
1:D:12:TYR:CE1	2:D:301:R3G:C6M	3.02	0.42
1:A:181:ILE:HD12	1:A:182:TRP:N	2.34	0.42
1:A:22:TYR:CD1	1:A:39:LYS:HG3	2.54	0.42
1:C:42:MET:HE1	1:C:206:PRO:HG3	2.01	0.42
1:D:112:THR:O	1:D:191:PHE:HA	2.19	0.42
1:C:204:SER:OG	1:C:205:HIS:CD2	2.70	0.42
2:C:301:R3G:H19	2:C:301:R3G:H21	1.34	0.42
1:D:25:ILE:O	1:D:37:THR:HA	2.20	0.42
1:B:229:LEU:HA	1:B:229:LEU:HD23	1.83	0.42
1:D:207:ALA:HA	1:D:208:ASP:HA	1.92	0.41
2:C:301:R3G:C5C	2:C:301:R3G:C14	2.98	0.41
1:C:111:PHE:CE2	1:C:113:SER:HB2	2.55	0.41
1:B:205:HIS:HA	1:B:206:PRO:HD2	1.70	0.41
1:C:107:LEU:HD11	1:C:198:LEU:HB2	2.02	0.41
1:D:53:ILE:HG22	1:D:192:GLU:HB2	2.03	0.41
1:C:170:VAL:HG21	1:C:231:GLY:HA2	2.03	0.41
1:A:42:MET:HE2	1:A:43:GLN:O	2.21	0.41
1:D:172:ARG:HD3	1:D:231:GLY:O	2.20	0.41
2:A:301:R3G:H7	2:A:301:R3G:H8	1.79	0.41
1:C:87:GLU:HG2	1:C:180:HIS:CD2	2.55	0.41
1:C:120:THR:O	1:C:120:THR:HG23	2.21	0.41
1:C:34:SER:HB2	1:C:37:THR:CG2	2.51	0.41
1:D:92:GLY:HA2	1:D:109:TRP:CH2	2.55	0.41
1:C:135:LYS:HG2	1:C:135:LYS:H	1.58	0.41
1:D:174:LEU:HD12	1:D:174:LEU:N	2.36	0.40
1:C:181:ILE:CD1	1:C:182:TRP:HD1	2.32	0.40
1:A:118:ASN:HB3	1:A:185:SER:HB2	2.03	0.40
1:C:54:TYR:HB3	1:C:191:PHE:CE2	2.56	0.40
1:B:116:LYS:CB	1:B:187:VAL:HG22	2.52	0.40
1:B:112:THR:O	1:B:191:PHE:HA	2.22	0.40
1:A:132:GLN:OE1	1:B:117:SER:HB3	2.22	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	235/237 (99%)	222 (94%)	11 (5%)	2 (1%)	21	10
1	B	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
1	C	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	39	28
1	D	235/237 (99%)	226 (96%)	9 (4%)	0	100	100
All	All	940/948 (99%)	896 (95%)	41 (4%)	3 (0%)	46	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	C	120	THR
1	A	21	SER

### 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	203/203 (100%)	196 (97%)	7 (3%)	44	37
1	B	203/203 (100%)	194 (96%)	9 (4%)	35	26
1	C	203/203 (100%)	198 (98%)	5 (2%)	55	49
1	D	203/203 (100%)	198 (98%)	5 (2%)	55	49
All	All	812/812 (100%)	786 (97%)	26 (3%)	46	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	115	LEU
1	A	117	SER
1	A	119	SER
1	A	120	THR
1	A	135	LYS
1	A	198	LEU
1	B	21	SER
1	B	66	SER
1	B	115	LEU
1	B	132	GLN
1	B	162	ASN
1	B	164	SER
1	B	192	GLU
1	B	198	LEU
1	B	223	SER
1	C	9	LEU
1	C	36	LYS
1	C	120	THR
1	C	132	GLN
1	C	135	LYS
1	D	82	ASP
1	D	116	LYS
1	D	135	LYS
1	D	166	GLN
1	D	198	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	166	GLN
1	A	205	HIS
1	A	237	ASN
1	B	43	GLN
1	B	121	HIS
1	B	205	HIS
1	B	237	ASN
1	C	43	GLN
1	C	121	HIS
1	C	166	GLN
1	C	205	HIS
1	C	237	ASN

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Mol	Chain	Res	Type
1	D	51	HIS
1	D	121	HIS
1	D	237	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](#)

Of 12 ligands modelled in this entry, 8 are 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	R3G	A	301	-	63,64,64	2.47	11 (17%)	81,88,88	2.02	22 (27%)
2	R3G	B	301	-	63,64,64	2.52	13 (20%)	81,88,88	1.85	18 (22%)
2	R3G	C	301	-	63,64,64	2.47	11 (17%)	81,88,88	2.26	22 (27%)
2	R3G	D	301	-	63,64,64	2.29	10 (15%)	81,88,88	1.98	21 (25%)

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	R3G	A	301	-	-	0/41/75/75	0/6/6/6
2	R3G	B	301	-	-	0/41/75/75	0/6/6/6
2	R3G	C	301	-	-	0/41/75/75	0/6/6/6
2	R3G	D	301	-	-	0/41/75/75	0/6/6/6

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	R3G	C1C-C2C	-9.48	1.37	1.52
2	B	301	R3G	C1C-C2C	-8.68	1.38	1.52
2	B	301	R3G	O1B-C4B	-8.14	1.25	1.38
2	A	301	R3G	O1B-C4B	-7.72	1.26	1.38
2	B	301	R3G	O1B-C1A	-7.66	1.26	1.38
2	C	301	R3G	O1B-C1A	-7.49	1.26	1.38
2	A	301	R3G	C2A-C2C	-7.37	1.40	1.52
2	D	301	R3G	O1B-C4B	-6.93	1.27	1.38
2	A	301	R3G	C1C-C2C	-6.74	1.41	1.52
2	B	301	R3G	C2A-C2C	-6.71	1.41	1.52
2	D	301	R3G	C2A-C2C	-6.60	1.41	1.52
2	D	301	R3G	O1B-C1A	-6.60	1.28	1.38
2	C	301	R3G	C2A-C2C	-6.37	1.42	1.52
2	A	301	R3G	O1B-C1A	-6.31	1.28	1.38
2	D	301	R3G	C1C-C2C	-5.46	1.43	1.52
2	C	301	R3G	O1B-C4B	-4.20	1.31	1.38
2	C	301	R3G	C2P-C2C	-2.74	1.49	1.53
2	B	301	R3G	C1P-C2P	-2.46	1.37	1.40
2	B	301	R3G	C2P-C2C	-2.32	1.50	1.53
2	D	301	R3G	C5T-N1T	2.06	1.36	1.33
2	D	301	R3G	C5C-C6C	2.07	1.42	1.38
2	C	301	R3G	C3C-C4C	2.20	1.43	1.39
2	A	301	R3G	C4T-C5T	2.28	1.39	1.36
2	A	301	R3G	C3P-C2P	2.29	1.42	1.39
2	B	301	R3G	C4A-C5A	2.43	1.44	1.39
2	C	301	R3G	C3C-C4B	2.45	1.43	1.38
2	B	301	R3G	C3P-C2P	2.55	1.43	1.39
2	B	301	R3G	C3A-C4A	2.55	1.43	1.38
2	A	301	R3G	N1T-N2T	2.76	1.38	1.34
2	A	301	R3G	O1M-C1M	2.91	1.45	1.40
2	D	301	R3G	N2T-N3T	2.97	1.40	1.34
2	B	301	R3G	N2T-N3T	3.05	1.40	1.34
2	C	301	R3G	N2T-N3T	3.84	1.41	1.34
2	B	301	R3G	C9-C8	3.86	1.59	1.51
2	D	301	R3G	N1T-N2T	4.04	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	R3G	O1-C7P	4.43	1.44	1.33
2	D	301	R3G	O1-C7P	4.61	1.44	1.33
2	A	301	R3G	N2T-N3T	4.64	1.43	1.34
2	C	301	R3G	N1T-N2T	4.65	1.41	1.34
2	C	301	R3G	O1-C7P	4.72	1.44	1.33
2	A	301	R3G	O1-C7P	5.61	1.46	1.33
2	B	301	R3G	C4T-N3T	6.44	1.42	1.35
2	D	301	R3G	C4T-N3T	8.03	1.44	1.35
2	A	301	R3G	C4T-N3T	8.43	1.45	1.35
2	C	301	R3G	C4T-N3T	8.43	1.45	1.35

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	R3G	C23-N1C-C4C	-6.16	112.23	121.42
2	C	301	R3G	C6C-C1C-C2C	-4.44	119.11	126.02
2	A	301	R3G	C21-N1A-C5A	-4.22	115.12	121.42
2	D	301	R3G	O1B-C4B-C1C	-3.97	119.47	122.54
2	B	301	R3G	O1B-C1A-C2A	-3.93	119.51	122.54
2	C	301	R3G	O7-C8-C9	-3.58	102.78	108.62
2	D	301	R3G	C3P-C2P-C1P	-3.58	114.18	118.72
2	C	301	R3G	C3C-C4B-C1C	-3.55	116.00	121.86
2	A	301	R3G	O1-C7P-O7P	-3.51	117.22	123.66
2	C	301	R3G	C4B-C1C-C2C	-3.31	117.12	120.80
2	D	301	R3G	C3A-C2A-C2C	-3.16	121.10	126.02
2	C	301	R3G	O1B-C1A-C2A	-3.14	120.11	122.54
2	C	301	R3G	C3C-C4C-N1C	-3.04	118.10	121.36
2	C	301	R3G	C3A-C2A-C2C	-2.99	121.37	126.02
2	A	301	R3G	O7-C8-C9	-2.95	103.81	108.62
2	B	301	R3G	C8-C9-N3T	-2.87	106.86	111.04
2	A	301	R3G	O4M-C4M-C3M	-2.86	103.89	110.34
2	B	301	R3G	C3P-C2P-C2C	-2.84	114.90	121.47
2	D	301	R3G	O7-C8-C9	-2.83	104.01	108.62
2	B	301	R3G	C4B-C1C-C2C	-2.81	117.67	120.80
2	D	301	R3G	O5M-C1M-C2M	-2.71	104.71	110.28
2	D	301	R3G	O1-C2-C3	-2.70	100.53	108.54
2	B	301	R3G	O4M-C4M-C3M	-2.69	104.29	110.34
2	A	301	R3G	O3M-C3M-C4M	-2.68	104.30	110.34
2	B	301	R3G	C3C-C4C-N1C	-2.63	118.53	121.36
2	A	301	R3G	C3A-C2A-C2C	-2.61	121.96	126.02
2	B	301	R3G	O3M-C3M-C4M	-2.58	104.52	110.34
2	C	301	R3G	O1-C7P-O7P	-2.56	118.95	123.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	R3G	C4B-C1C-C2C	-2.50	118.02	120.80
2	D	301	R3G	O2M-C2M-C1M	-2.47	104.60	110.02
2	A	301	R3G	O1B-C1A-C2A	-2.40	120.68	122.54
2	B	301	R3G	C13-N1C-C4C	-2.17	118.19	121.42
2	C	301	R3G	C21-N1A-C5A	-2.11	118.27	121.42
2	D	301	R3G	C11-N1A-C5A	-2.01	118.43	121.42
2	A	301	R3G	C2P-C1P-C7P	2.05	125.73	122.15
2	D	301	R3G	C13-N1C-C4C	2.06	124.50	121.42
2	A	301	R3G	O1-C2-C3	2.11	114.81	108.54
2	D	301	R3G	C11-N1A-C21	2.13	120.24	116.29
2	B	301	R3G	C11-N1A-C5A	2.17	124.66	121.42
2	A	301	R3G	O4M-C4M-C5M	2.24	115.17	109.24
2	C	301	R3G	O1-C7P-C1P	2.25	116.26	112.16
2	D	301	R3G	N1T-N2T-N3T	2.26	109.02	107.31
2	B	301	R3G	C13-N1C-C23	2.26	120.48	116.29
2	A	301	R3G	O1M-C1M-C2M	2.34	110.99	108.04
2	C	301	R3G	C24-C23-N1C	2.34	123.99	112.13
2	D	301	R3G	C3C-C4C-N1C	2.38	123.93	121.36
2	C	301	R3G	C11-N1A-C21	2.43	120.79	116.29
2	A	301	R3G	O1B-C4B-C3C	2.46	119.34	115.34
2	A	301	R3G	C4B-O1B-C1A	2.48	124.34	118.53
2	B	301	R3G	C4B-O1B-C1A	2.51	124.41	118.53
2	D	301	R3G	C4B-O1B-C1A	2.62	124.69	118.53
2	B	301	R3G	C3A-C4A-C5A	2.64	123.77	120.36
2	D	301	R3G	C6C-C5C-C4C	2.76	123.93	120.36
2	A	301	R3G	O1B-C1A-C6A	2.81	119.90	115.34
2	A	301	R3G	C6A-C5A-N1A	2.88	124.46	121.36
2	B	301	R3G	O3M-C3M-C2M	2.95	116.97	110.34
2	C	301	R3G	O1M-C1M-C2M	3.02	111.86	108.04
2	A	301	R3G	C11-N1A-C21	3.18	122.18	116.29
2	D	301	R3G	O1-C7P-C1P	3.20	117.99	112.16
2	A	301	R3G	O1-C7P-C1P	3.35	118.25	112.16
2	B	301	R3G	O1-C7P-C1P	3.54	118.60	112.16
2	D	301	R3G	O1M-C1M-C2M	3.57	112.55	108.04
2	C	301	R3G	O1B-C1A-C6A	3.60	121.18	115.34
2	B	301	R3G	C2P-C2C-C2A	3.68	120.01	112.71
2	C	301	R3G	C2P-C2C-C1C	3.70	120.05	112.71
2	C	301	R3G	O1B-C4B-C3C	3.83	121.56	115.34
2	D	301	R3G	C6P-C1P-C2P	3.84	124.05	119.54
2	C	301	R3G	C2-O1-C7P	4.06	125.03	116.42
2	B	301	R3G	C2-O1-C7P	4.11	125.15	116.42
2	D	301	R3G	C2P-C2C-C2A	4.12	120.87	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	R3G	C13-N1C-C23	4.16	123.99	116.29
2	A	301	R3G	C2-O1-C7P	4.26	125.48	116.42
2	C	301	R3G	C2P-C2C-C2A	4.39	121.42	112.71
2	A	301	R3G	C2P-C2C-C2A	4.43	121.50	112.71
2	A	301	R3G	C2P-C2C-C1C	4.54	121.72	112.71
2	C	301	R3G	C6C-C1C-C4B	5.09	123.77	117.76
2	B	301	R3G	C2P-C2C-C1C	5.15	122.91	112.71
2	D	301	R3G	C2-O1-C7P	5.18	127.43	116.42
2	D	301	R3G	C1C-C2C-C2A	5.34	113.81	105.87
2	D	301	R3G	C2P-C2C-C1C	6.33	125.27	112.71
2	A	301	R3G	C1C-C2C-C2A	7.34	116.78	105.87
2	B	301	R3G	C1C-C2C-C2A	7.51	117.05	105.87
2	C	301	R3G	C1C-C2C-C2A	8.51	118.53	105.87

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
2	A	301	R3G	2	0
2	B	301	R3G	1	0
2	C	301	R3G	5	0
2	D	301	R3G	5	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, 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	237/237 (100%)	-0.23	2 (0%) 87 89	18, 29, 54, 74	0
1	B	237/237 (100%)	-0.14	4 (1%) 73 76	24, 33, 56, 76	0
1	C	237/237 (100%)	-0.17	4 (1%) 73 76	19, 30, 52, 80	0
1	D	237/237 (100%)	-0.07	4 (1%) 73 76	23, 33, 57, 73	0
All	All	948/948 (100%)	-0.16	14 (1%) 76 79	18, 31, 55, 80	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	THR	10.0
1	B	120	THR	4.5
1	D	120	THR	4.1
1	D	185	SER	4.1
1	D	119	SER	3.7
1	A	120	THR	3.6
1	B	119	SER	3.2
1	C	150	THR	2.8
1	A	185	SER	2.7
1	B	162	ASN	2.4
1	B	185	SER	2.3
1	C	151	ASP	2.1
1	D	150	THR	2.1
1	C	118	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 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(Å <sup>2</sup> )	Q<0.9
3	MN	B	302	1/1	0.98	0.11	1.85	35,35,35,35	0
2	R3G	B	301	59/59	0.95	0.12	1.36	27,40,49,52	0
4	CA	B	303	1/1	0.99	0.12	1.28	33,33,33,33	0
2	R3G	A	301	59/59	0.96	0.12	1.21	23,38,51,53	0
2	R3G	C	301	59/59	0.96	0.11	0.32	23,29,40,43	0
2	R3G	D	301	59/59	0.95	0.11	0.27	26,34,38,41	0
3	MN	D	302	1/1	0.99	0.10	0.09	34,34,34,34	0
3	MN	C	302	1/1	0.99	0.10	-0.05	29,29,29,29	0
3	MN	A	302	1/1	0.99	0.10	-0.32	30,30,30,30	0
4	CA	A	303	1/1	0.99	0.10	-0.34	26,26,26,26	0
4	CA	D	303	1/1	0.99	0.09	-0.67	30,30,30,30	0
4	CA	C	303	1/1	1.00	0.07	-2.88	28,28,28,28	0

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

There are no such residues in this entry.