



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:00 AM GMT

PDB ID : 2P2K  
Title : Crystal structure of a lectin from Canavalia gladiata seeds (CGL) in complex with man1-4man-OMe  
Authors : Moreno, F.B.M.B.; Bezerra, G.A.; Oliveira, T.M.; Souza, E.P.; Rocha, B.A.M.; Benevides, G.B.; Delatorre, P.; Cavada, B.S.; de Azevedo Jr., W.F.  
Deposited on : 2007-03-07  
Resolution : 1.98 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

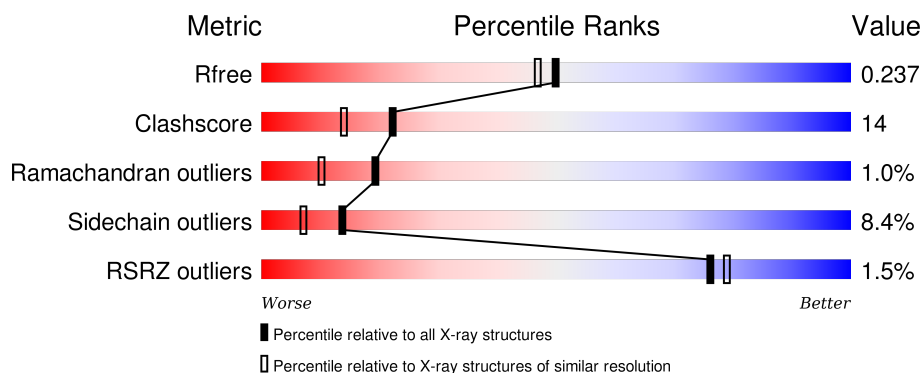
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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>76%</div> <div>20%</div> <div>...</div> </div>
1	B	237	<div> <div>73%</div> <div>22%</div> <div>...</div> </div>
1	C	237	<div> <div>67%</div> <div>29%</div> <div>...</div> </div>
1	D	237	<div> <div>64%</div> <div>28%</div> <div>6%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MMA	O	240	X	-	-	X
2	MMA	P	242	X	-	-	-
2	MMA	Q	244	X	-	-	-
2	MMA	R	246	X	-	-	X
3	MN	B	238	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7697 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 Canavalia gladiata lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1779	1123	298	356	2			
1	B	234	Total	C	N	O	S	0	0	0
			1782	1125	298	357	2			
1	C	234	Total	C	N	O	S	0	0	0
			1779	1123	298	356	2			
1	D	234	Total	C	N	O	S	0	0	0
			1782	1125	298	357	2			

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	2	Total	C	O	0	0
			24	13	11		
2	P	2	Total	C	O	0	0
			24	13	11		
2	Q	2	Total	C	O	0	0
			24	13	11		
2	R	2	Total	C	O	0	0
			24	13	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 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

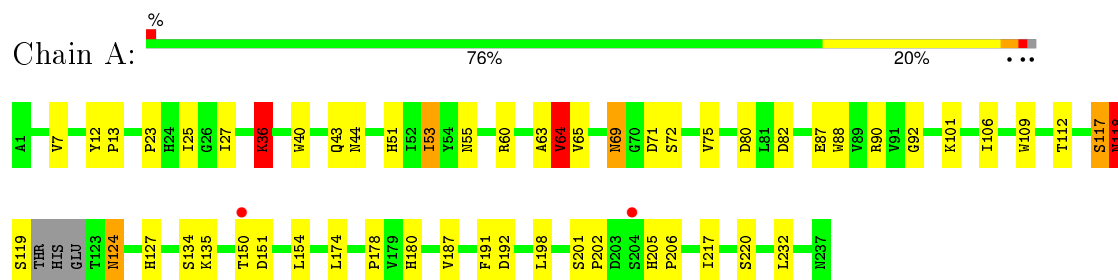
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	149	Total 149	O 149	0	0
5	B	142	Total 142	O 142	0	0
5	C	82	Total 82	O 82	0	0
5	D	89	Total 89	O 89	0	0
5	O	2	Total 2	O 2	0	0
5	P	3	Total 3	O 3	0	0
5	Q	3	Total 3	O 3	0	0
5	R	1	Total 1	O 1	0	0

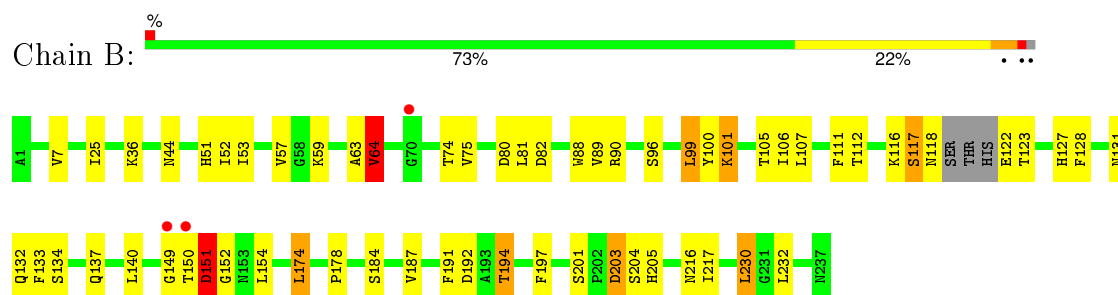
### 3 Residue-property plots

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.

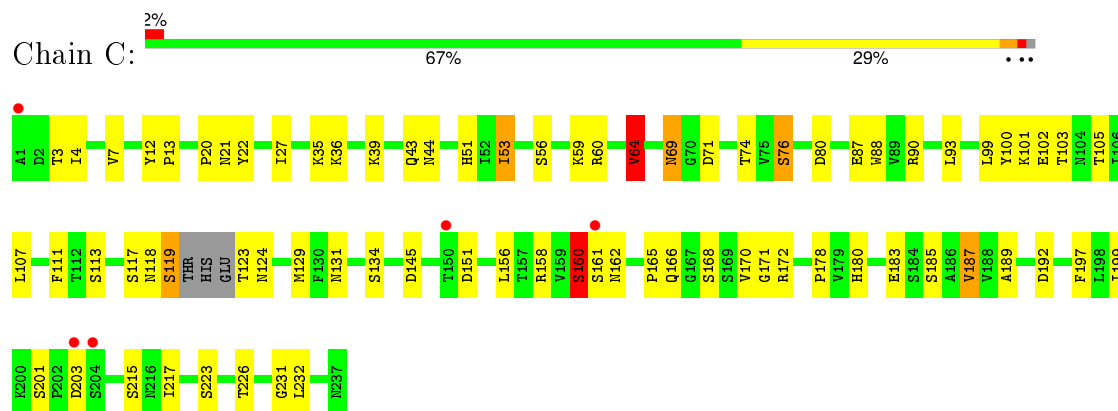
- Molecule 1: *Canavalia gladiata* lectin



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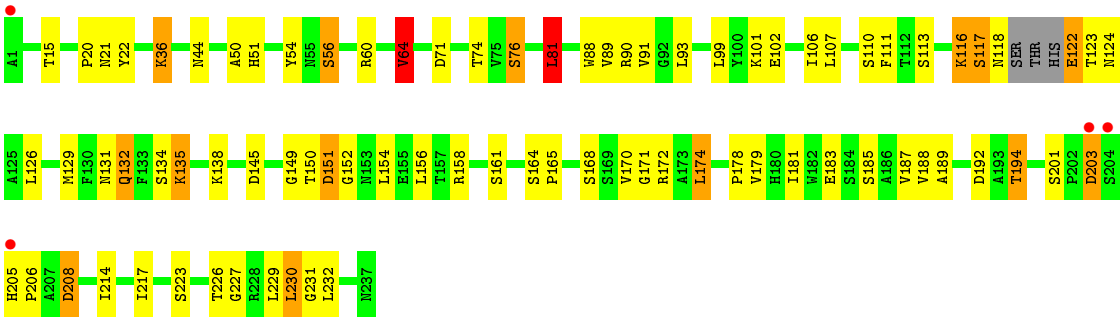


- Molecule 1: *Canavalia gladiata* lectin



- Molecule 1: *Canavalia gladiata* lectin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.93Å 68.93Å 160.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.84 – 1.98 39.83 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.84-1.98) 99.5 (39.83-1.98)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	6.80	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.182 , 0.236 0.184 , 0.237	Depositor DCC
$R_{free}$ test set	2983 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 18.4	EDS
Estimated twinning fraction	0.027 for -h,-k,l 0.486 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 59097 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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, MN, MMA, MAN

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	0.92	2/1819 (0.1%)	0.97	4/2476 (0.2%)
1	B	0.95	2/1822 (0.1%)	1.02	6/2480 (0.2%)
1	C	0.92	1/1820 (0.1%)	1.12	6/2479 (0.2%)
1	D	0.86	2/1822 (0.1%)	1.01	10/2480 (0.4%)
All	All	0.91	7/7283 (0.1%)	1.03	26/9915 (0.3%)

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	B	0	2
1	C	0	1
1	D	0	1
2	O	1	0
2	P	1	0
2	Q	1	0
2	R	1	0
All	All	4	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	SER	C-N	18.07	1.75	1.34
1	B	101	LYS	CE-NZ	7.33	1.67	1.49
1	D	36	LYS	CE-NZ	6.54	1.65	1.49
1	D	36	LYS	CB-CG	6.53	1.70	1.52
1	B	89	VAL	CB-CG1	5.69	1.64	1.52
1	A	36	LYS	CE-NZ	5.19	1.62	1.49
1	A	36	LYS	CD-CE	5.10	1.64	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	SER	O-C-N	-24.89	82.87	122.70
1	C	119	SER	CA-C-N	16.08	152.57	117.20
1	C	119	SER	C-N-CA	10.68	148.39	121.70
1	D	230	LEU	N-CA-C	-10.22	83.40	111.00
1	D	36	LYS	CD-CE-NZ	9.30	133.09	111.70
1	C	64	VAL	CB-CA-C	-8.54	95.17	111.40
1	D	229	LEU	C-N-CA	8.32	142.50	121.70
1	A	64	VAL	CB-CA-C	-8.29	95.65	111.40
1	D	64	VAL	CB-CA-C	-8.01	96.18	111.40
1	B	64	VAL	CB-CA-C	-7.82	96.55	111.40
1	D	174	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	64	VAL	CG1-CB-CG2	7.26	122.52	110.90
1	B	151	ASP	N-CA-C	7.19	130.40	111.00
1	B	174	LEU	CA-CB-CG	7.12	131.68	115.30
1	D	229	LEU	O-C-N	-6.78	111.86	122.70
1	C	64	VAL	CG1-CB-CG2	6.15	120.74	110.90
1	D	64	VAL	CG1-CB-CG2	5.99	120.48	110.90
1	D	229	LEU	CA-C-N	5.95	130.29	117.20
1	D	229	LEU	N-CA-C	5.91	126.94	111.00
1	B	151	ASP	N-CA-CB	-5.80	100.16	110.60
1	D	81	LEU	CB-CG-CD1	5.68	120.65	111.00
1	A	60	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	60	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	21	ASN	CB-CA-C	5.33	121.05	110.40
1	B	64	VAL	CG1-CB-CG2	5.10	119.05	110.90
1	B	101	LYS	CD-CE-NZ	-5.03	100.13	111.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	O	240	MMA	C1
2	P	242	MMA	C1
2	Q	244	MMA	C1
2	R	246	MMA	C1

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	LYS	Peptide
1	B	149	GLY	Peptide
1	C	160	SER	Peptide

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Mol	Chain	Res	Type	Group
1	D	116	LYS	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	1779	0	1730	42	0
1	B	1782	0	1731	48	0
1	C	1779	0	1730	56	0
1	D	1782	0	1730	62	1
2	O	24	0	23	1	0
2	P	24	0	23	0	0
2	Q	24	0	23	0	0
2	R	24	0	23	2	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	149	0	0	5	0
5	B	142	0	0	6	0
5	C	82	0	0	8	0
5	D	89	0	0	6	0
5	O	2	0	0	1	0
5	P	3	0	0	0	1
5	Q	3	0	0	0	0
5	R	1	0	0	0	0
All	All	7697	0	7013	196	1

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 14.

All (196) 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:119:SER:C	1:C:123:THR:N	1.75	1.36
1:D:150:THR:HA	1:D:152:GLY:H	1.00	1.12
1:B:150:THR:HA	1:B:152:GLY:H	0.96	1.10
1:B:64:VAL:HG13	1:B:74:THR:HG22	1.33	1.09
1:A:53:ILE:CD1	5:C:300:HOH:O	2.02	1.08
1:D:64:VAL:HG13	1:D:74:THR:HG22	1.34	1.06
1:D:117:SER:HB3	1:D:118:ASN:HA	1.05	1.02
1:B:150:THR:HA	1:B:152:GLY:N	1.76	1.00
1:B:203:ASP:O	1:B:205:HIS:N	1.96	0.96
1:D:117:SER:HB3	1:D:118:ASN:CA	1.95	0.95
1:B:74:THR:HG23	5:B:366:HOH:O	1.62	0.95
1:D:117:SER:CB	1:D:118:ASN:HA	1.95	0.94
1:A:53:ILE:HD11	5:C:300:HOH:O	1.67	0.93
1:C:119:SER:O	1:C:123:THR:N	2.02	0.91
1:D:150:THR:HA	1:D:152:GLY:N	1.85	0.90
1:A:205:HIS:HD2	1:A:206:PRO:O	1.55	0.89
1:C:44:ASN:HD21	1:C:201:SER:H	1.20	0.88
1:A:118:ASN:HB3	5:A:360:HOH:O	1.73	0.88
1:B:134:SER:H	1:B:137:GLN:NE2	1.76	0.83
1:B:117:SER:CB	1:B:118:ASN:HA	2.08	0.82
1:A:118:ASN:OD1	1:A:119:SER:N	2.13	0.81
1:D:150:THR:CA	1:D:152:GLY:H	1.90	0.81
1:A:205:HIS:CD2	1:A:206:PRO:O	2.34	0.81
1:C:88:TRP:HB3	1:C:217:ILE:HD11	1.62	0.81
1:A:44:ASN:HD21	1:A:201:SER:H	1.27	0.81
1:D:99:LEU:HD12	2:O:240:MMA:H4	1.61	0.81
1:B:194:THR:HG22	5:B:316:HOH:O	1.83	0.78
1:A:51:HIS:HB2	1:A:64:VAL:HG23	1.64	0.77
1:C:166:GLN:HG3	5:C:315:HOH:O	1.84	0.77
1:D:44:ASN:HD21	1:D:201:SER:H	1.36	0.74
1:A:36:LYS:HD2	1:A:75:VAL:HG23	1.70	0.74
1:A:124:ASN:HD21	1:B:132:GLN:H	1.35	0.73
1:B:117:SER:HB3	1:B:118:ASN:HA	1.69	0.73
1:B:194:THR:CG2	5:B:316:HOH:O	2.35	0.73
1:B:36:LYS:HE3	5:B:272:HOH:O	1.90	0.72
1:B:203:ASP:C	1:B:205:HIS:H	1.92	0.72
1:D:150:THR:HB	1:D:151:ASP:HA	1.70	0.72
1:C:53:ILE:C	1:C:53:ILE:HD13	2.10	0.71
1:B:117:SER:HB2	1:B:187:VAL:HG12	1.70	0.71
1:A:53:ILE:HD12	5:C:300:HOH:O	1.78	0.71
1:C:107:LEU:O	5:C:321:HOH:O	2.11	0.68
1:A:44:ASN:HD21	1:A:201:SER:N	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:HIS:HD2	1:D:206:PRO:O	1.77	0.68
1:B:80:ASP:OD1	1:B:82:ASP:HB2	1.95	0.66
1:A:117:SER:HA	1:A:187:VAL:HG22	1.78	0.66
1:B:64:VAL:HG13	1:B:74:THR:CG2	2.21	0.66
1:A:90:ARG:NH1	1:A:217:ILE:HG23	2.11	0.65
1:C:124:ASN:ND2	1:D:131:ASN:H	1.94	0.65
1:B:99:LEU:HD13	1:B:100:TYR:CZ	2.32	0.65
1:A:178:PRO:HB3	1:A:217:ILE:CD1	2.27	0.64
1:D:122:GLU:HG2	5:D:310:HOH:O	1.98	0.64
1:C:131:ASN:O	5:C:321:HOH:O	2.15	0.64
1:C:156:LEU:O	1:C:171:GLY:HA3	1.98	0.63
1:C:51:HIS:HB2	1:C:64:VAL:HG23	1.81	0.63
1:D:44:ASN:ND2	1:D:201:SER:H	1.96	0.63
5:B:352:HOH:O	1:D:194:THR:HG21	1.97	0.63
1:C:160:SER:O	1:C:162:ASN:N	2.31	0.63
1:B:134:SER:H	1:B:137:GLN:HE21	1.46	0.63
1:D:122:GLU:CG	5:D:310:HOH:O	2.48	0.62
1:B:51:HIS:HB2	1:B:64:VAL:HG23	1.82	0.62
1:D:36:LYS:HE3	5:D:243:HOH:O	1.98	0.62
1:D:51:HIS:HB2	1:D:64:VAL:HG23	1.80	0.61
1:C:88:TRP:HB3	1:C:217:ILE:CD1	2.28	0.61
1:D:178:PRO:HB3	1:D:217:ILE:HD11	1.82	0.61
1:C:7:VAL:HG22	1:C:27:ILE:CD1	2.32	0.60
1:C:56:SER:CB	1:C:189:ALA:H	2.15	0.59
1:B:117:SER:HB3	1:B:118:ASN:CA	2.32	0.59
1:B:53:ILE:HD13	5:D:292:HOH:O	2.01	0.59
1:D:201:SER:OG	1:D:203:ASP:HB2	2.03	0.59
1:D:20:PRO:HB2	1:D:22:TYR:CZ	2.38	0.58
1:B:194:THR:HG21	5:D:306:HOH:O	2.02	0.58
1:A:25:ILE:HD12	1:A:75:VAL:HG12	1.86	0.58
1:D:88:TRP:HB3	1:D:217:ILE:CD1	2.34	0.57
1:A:88:TRP:HB3	1:A:217:ILE:HD11	1.87	0.57
1:A:151:ASP:HB2	5:A:361:HOH:O	2.05	0.57
1:C:53:ILE:O	1:C:53:ILE:HD13	2.04	0.56
1:D:99:LEU:HD12	5:O:242:HOH:O	2.05	0.56
1:A:36:LYS:HD2	1:A:75:VAL:CG2	2.34	0.56
1:D:64:VAL:HG13	1:D:74:THR:CG2	2.22	0.56
1:B:88:TRP:HB3	1:B:217:ILE:HD11	1.87	0.56
1:B:25:ILE:HD12	1:B:75:VAL:HG12	1.86	0.56
1:C:20:PRO:HB2	1:C:22:TYR:CZ	2.41	0.56
1:B:137:GLN:HG2	1:B:140:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASN:HD21	1:C:71:ASP:HB2	1.71	0.56
1:B:134:SER:N	1:B:137:GLN:NE2	2.52	0.55
1:B:44:ASN:HD21	1:B:201:SER:H	1.52	0.55
1:B:44:ASN:HD21	1:B:201:SER:N	2.04	0.55
1:C:145:ASP:HB3	1:C:158:ARG:HG2	1.88	0.55
1:D:56:SER:CB	1:D:189:ALA:H	2.20	0.55
1:D:111:PHE:CE2	1:D:113:SER:HB2	2.42	0.55
1:D:88:TRP:HB3	1:D:217:ILE:HD11	1.89	0.55
1:C:60:ARG:HD3	1:C:76:SER:OG	2.07	0.55
1:C:100:TYR:HD2	2:R:247:MAN:H62	1.71	0.55
1:D:60:ARG:HD3	1:D:76:SER:OG	2.07	0.55
1:A:178:PRO:HB3	1:A:217:ILE:HD11	1.88	0.55
1:B:90:ARG:NH1	1:B:217:ILE:CG2	2.70	0.54
1:A:44:ASN:ND2	1:A:201:SER:H	2.02	0.54
1:A:151:ASP:CB	5:A:361:HOH:O	2.56	0.54
1:C:44:ASN:ND2	1:C:201:SER:H	1.97	0.53
1:D:90:ARG:NH1	1:D:217:ILE:HG23	2.24	0.52
1:D:145:ASP:HB3	1:D:158:ARG:HG2	1.91	0.52
1:A:124:ASN:ND2	1:B:131:ASN:H	2.07	0.52
1:D:178:PRO:HB3	1:D:217:ILE:CD1	2.39	0.52
1:B:178:PRO:HB3	1:B:217:ILE:CD1	2.40	0.51
1:A:43:GLN:HE22	1:A:69:ASN:HD21	1.57	0.51
1:D:156:LEU:O	1:D:171:GLY:HA3	2.10	0.51
1:C:99:LEU:HD22	2:R:246:MMA:H4	1.92	0.51
1:C:59:LYS:HD3	1:C:80:ASP:HB2	1.92	0.51
1:C:35:LYS:O	1:C:36:LYS:HG2	2.10	0.51
1:D:116:LYS:O	1:D:187:VAL:N	2.44	0.50
1:C:90:ARG:NH1	1:C:217:ILE:HG23	2.26	0.50
1:A:127:HIS:HB3	1:B:127:HIS:HB3	1.93	0.50
1:C:4:ILE:HD13	1:C:215:SER:HB3	1.93	0.50
1:C:43:GLN:HE22	1:C:69:ASN:ND2	2.09	0.50
1:B:99:LEU:HD13	1:B:100:TYR:CE2	2.46	0.49
1:A:112:THR:O	1:A:191:PHE:HA	2.11	0.49
1:B:105:THR:O	1:B:197:PHE:HA	2.12	0.49
1:B:90:ARG:NH1	1:B:217:ILE:HG22	2.27	0.49
1:B:122:GLU:OE2	1:B:123:THR:OG1	2.31	0.49
1:C:102:GLU:C	1:C:165:PRO:HB3	2.33	0.49
1:C:119:SER:HB3	1:D:131:ASN:HB3	1.95	0.48
1:D:54:TYR:CE1	1:D:81:LEU:HD22	2.48	0.48
1:C:124:ASN:HD21	1:D:132:GLN:H	1.61	0.48
5:A:327:HOH:O	1:C:74:THR:HG21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:SER:HB3	5:C:295:HOH:O	2.12	0.48
1:D:91:VAL:HG12	1:D:214:ILE:HG12	1.95	0.48
1:B:96:SER:OG	1:B:230:LEU:HA	2.13	0.48
1:C:187:VAL:HG11	5:C:292:HOH:O	2.13	0.48
1:D:170:VAL:HG21	1:D:231:GLY:HA2	1.94	0.48
1:D:170:VAL:HB	1:D:226:THR:HG22	1.96	0.48
1:A:51:HIS:O	1:A:63:ALA:HA	2.14	0.47
1:A:69:ASN:HD21	1:A:71:ASP:HB3	1.79	0.47
1:C:170:VAL:HB	1:C:226:THR:HG22	1.97	0.47
1:B:7:VAL:HG21	1:B:52:ILE:HG12	1.96	0.47
1:B:57:VAL:HG21	1:D:64:VAL:HG22	1.96	0.46
1:D:54:TYR:CD1	1:D:81:LEU:HD22	2.51	0.46
1:C:12:TYR:HA	1:C:13:PRO:HD3	1.77	0.46
1:B:118:ASN:OD1	5:B:367:HOH:O	2.21	0.46
1:A:7:VAL:HG22	1:A:27:ILE:HD12	1.97	0.46
1:D:110:SER:HB3	1:D:129:MET:HG3	1.98	0.46
1:C:43:GLN:HE22	1:C:69:ASN:HD21	1.63	0.46
1:A:92:GLY:HA2	1:A:109:TRP:CH2	2.50	0.46
1:C:158:ARG:HB2	1:C:166:GLN:HB3	1.98	0.46
1:C:178:PRO:HB3	1:C:217:ILE:CD1	2.46	0.45
1:C:217:ILE:CD1	1:D:138:LYS:HD2	2.46	0.45
1:A:12:TYR:HA	1:A:13:PRO:HD3	1.83	0.45
1:A:80:ASP:OD1	1:A:82:ASP:HB2	2.17	0.45
1:B:133:PHE:HA	1:B:137:GLN:NE2	2.31	0.45
1:C:22:TYR:CD2	1:C:39:LYS:HE3	2.52	0.45
1:C:111:PHE:CE2	1:C:113:SER:HB2	2.51	0.45
1:C:107:LEU:HD12	1:C:107:LEU:N	2.31	0.45
1:A:69:ASN:ND2	1:A:71:ASP:H	2.15	0.45
1:D:205:HIS:CD2	1:D:206:PRO:O	2.65	0.44
1:D:102:GLU:C	1:D:165:PRO:HB3	2.38	0.44
1:C:36:LYS:HE3	1:C:76:SER:O	2.18	0.44
1:B:112:THR:O	1:B:191:PHE:HA	2.18	0.43
1:A:106:ILE:HB	1:A:154:LEU:HB3	2.00	0.43
1:A:174:LEU:N	1:A:174:LEU:HD12	2.32	0.43
1:D:208:ASP:OD2	1:D:227:GLY:HA2	2.19	0.43
1:B:51:HIS:O	1:B:63:ALA:HA	2.19	0.43
1:C:87:GLU:HG3	1:C:180:HIS:CD2	2.54	0.43
1:D:106:ILE:HB	1:D:154:LEU:HB3	2.01	0.43
1:D:15:THR:HG21	1:D:21:ASN:HD22	1.84	0.43
1:D:116:LYS:HG3	1:D:188:VAL:HB	2.01	0.43
1:C:105:THR:O	1:C:197:PHE:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:MET:HE3	1:D:123:THR:HB	2.01	0.42
1:A:90:ARG:NH1	1:A:217:ILE:CG2	2.80	0.42
1:D:88:TRP:HB3	1:D:217:ILE:HD12	2.01	0.42
1:D:50:ALA:O	1:D:194:THR:HA	2.20	0.42
5:A:315:HOH:O	1:C:118:ASN:HA	2.20	0.42
1:A:65:VAL:O	1:A:72:SER:HA	2.20	0.42
1:C:170:VAL:HG21	1:C:231:GLY:HA2	2.00	0.42
1:D:126:LEU:CD2	1:D:179:VAL:HG22	2.49	0.42
1:C:53:ILE:C	1:C:53:ILE:CD1	2.84	0.42
1:C:124:ASN:HA	1:D:129:MET:O	2.20	0.42
1:A:69:ASN:C	1:A:69:ASN:HD22	2.22	0.42
1:A:198:LEU:HD23	1:A:198:LEU:C	2.39	0.41
1:D:135:LYS:HG3	1:D:149:GLY:O	2.20	0.41
1:B:59:LYS:HD3	1:B:80:ASP:HA	2.02	0.41
1:D:150:THR:CB	1:D:151:ASP:HA	2.44	0.41
1:D:149:GLY:HA2	1:D:150:THR:O	2.21	0.41
1:A:55:ASN:HD21	1:C:53:ILE:HD12	1.85	0.41
1:A:87:GLU:HG2	1:A:180:HIS:CD2	2.55	0.41
1:C:93:LEU:O	1:C:172:ARG:HA	2.21	0.41
1:D:93:LEU:O	1:D:172:ARG:HA	2.20	0.41
1:C:103:THR:O	1:C:199:ILE:HA	2.20	0.41
1:C:3:THR:O	1:C:215:SER:HA	2.21	0.41
1:D:15:THR:CG2	1:D:21:ASN:HD22	2.33	0.41
1:B:106:ILE:HB	1:B:154:LEU:HB3	2.02	0.40
1:D:89:VAL:HG22	1:D:181:ILE:HB	2.03	0.40
1:B:187:VAL:HG21	5:D:299:HOH:O	2.21	0.40
1:D:107:LEU:N	1:D:107:LEU:HD12	2.36	0.40
1:B:64:VAL:CG1	1:B:74:THR:HG22	2.25	0.40
1:C:129:MET:O	1:D:124:ASN:HA	2.20	0.40
1:B:111:PHE:HB3	1:B:128:PHE:CZ	2.56	0.40
1:A:23:PRO:HB2	1:A:40:TRP:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:SER:CB	5:P:246:HOH:O[2_664]	1.29	0.91



## 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	230/237 (97%)	219 (95%)	9 (4%)	2 (1%)	21	12
1	B	230/237 (97%)	219 (95%)	8 (4%)	3 (1%)	15	6
1	C	232/237 (98%)	219 (94%)	11 (5%)	2 (1%)	21	12
1	D	230/237 (97%)	219 (95%)	9 (4%)	2 (1%)	21	12
All	All	922/948 (97%)	876 (95%)	37 (4%)	9 (1%)	19	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	ASP
1	B	204	SER
1	C	161	SER
1	C	203	ASP
1	D	203	ASP
1	B	203	ASP
1	A	202	PRO
1	D	151	ASP
1	A	118	ASN

### 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	199/202 (98%)	185 (93%)	14 (7%)	19	11
1	B	199/202 (98%)	185 (93%)	14 (7%)	19	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	199/202 (98%)	183 (92%)	16 (8%)	15	8
1	D	199/202 (98%)	176 (88%)	23 (12%)	7	3
All	All	796/808 (98%)	729 (92%)	67 (8%)	14	7

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	53	ILE
1	A	64	VAL
1	A	69	ASN
1	A	101	LYS
1	A	117	SER
1	A	118	ASN
1	A	124	ASN
1	A	134	SER
1	A	135	LYS
1	A	150	THR
1	A	192	ASP
1	A	220	SER
1	A	232	LEU
1	B	64	VAL
1	B	81	LEU
1	B	99	LEU
1	B	101	LYS
1	B	107	LEU
1	B	117	SER
1	B	151	ASP
1	B	174	LEU
1	B	184	SER
1	B	192	ASP
1	B	194	THR
1	B	216	ASN
1	B	230	LEU
1	B	232	LEU
1	C	53	ILE
1	C	64	VAL
1	C	69	ASN
1	C	76	SER
1	C	101	LYS
1	C	117	SER

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Mol	Chain	Res	Type
1	C	134	SER
1	C	151	ASP
1	C	160	SER
1	C	168	SER
1	C	183	GLU
1	C	185	SER
1	C	187	VAL
1	C	192	ASP
1	C	223	SER
1	C	232	LEU
1	D	56	SER
1	D	64	VAL
1	D	71	ASP
1	D	76	SER
1	D	81	LEU
1	D	101	LYS
1	D	117	SER
1	D	122	GLU
1	D	132	GLN
1	D	134	SER
1	D	135	LYS
1	D	161	SER
1	D	164	SER
1	D	168	SER
1	D	174	LEU
1	D	183	GLU
1	D	185	SER
1	D	192	ASP
1	D	194	THR
1	D	208	ASP
1	D	223	SER
1	D	230	LEU
1	D	232	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	41	ASN
1	A	44	ASN
1	A	69	ASN
1	A	83	ASN

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	124	ASN
1	A	166	GLN
1	A	205	HIS
1	B	41	ASN
1	B	44	ASN
1	B	104	ASN
1	B	118	ASN
1	B	137	GLN
1	B	166	GLN
1	C	41	ASN
1	C	44	ASN
1	C	69	ASN
1	C	124	ASN
1	C	131	ASN
1	D	21	ASN
1	D	44	ASN
1	D	104	ASN
1	D	132	GLN
1	D	205	HIS

### 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](#)

8 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
2	MMA	O	240	2	13,13,13	0.94	1 (7%)	18,18,18	1.27	3 (16%)
2	MAN	O	241	2	11,11,12	1.03	1 (9%)	14,15,17	1.28	2 (14%)
2	MMA	P	242	2	13,13,13	0.60	0	18,18,18	3.76	7 (38%)
2	MAN	P	243	2	11,11,12	0.70	0	14,15,17	1.45	2 (14%)
2	MMA	Q	244	2	13,13,13	0.67	0	18,18,18	3.79	7 (38%)
2	MAN	Q	245	2	11,11,12	0.81	0	14,15,17	1.66	2 (14%)
2	MMA	R	246	2	13,13,13	0.97	1 (7%)	18,18,18	1.38	2 (11%)
2	MAN	R	247	2	11,11,12	0.97	1 (9%)	14,15,17	1.19	2 (14%)

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	MMA	O	240	2	1/1/5/5	0/4/24/24	0/1/1/1
2	MAN	O	241	2	-	0/2/19/22	0/1/1/1
2	MMA	P	242	2	1/1/5/5	0/4/24/24	0/1/1/1
2	MAN	P	243	2	-	0/2/19/22	0/1/1/1
2	MMA	Q	244	2	1/1/5/5	0/4/24/24	0/1/1/1
2	MAN	Q	245	2	-	0/2/19/22	0/1/1/1
2	MMA	R	246	2	1/1/5/5	0/4/24/24	0/1/1/1
2	MAN	R	247	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	247	MAN	C2-C3	2.30	1.55	1.52
2	R	246	MMA	O1-C1	2.47	1.44	1.40
2	O	240	MMA	O1-C1	2.56	1.44	1.40
2	O	241	MAN	C2-C3	2.67	1.56	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	242	MMA	C1-C2-C3	-7.66	94.88	109.97
2	Q	244	MMA	C1-C2-C3	-7.57	95.05	109.97
2	P	242	MMA	C1-O5-C5	-7.55	99.09	113.75
2	Q	244	MMA	C1-O5-C5	-7.05	100.05	113.75
2	P	242	MMA	O6-C6-C5	-4.04	97.97	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	243	MAN	O2-C2-C1	-2.97	103.26	109.21
2	Q	244	MMA	O2-C2-C3	-2.72	104.22	110.34
2	Q	244	MMA	O6-C6-C5	-2.68	102.48	111.33
2	O	240	MMA	O5-C1-C2	-2.24	105.67	110.28
2	Q	245	MAN	O3-C3-C2	-2.24	105.95	110.00
2	R	246	MMA	C1-O5-C5	2.07	117.75	113.75
2	R	247	MAN	O2-C2-C3	2.10	114.34	110.12
2	R	247	MAN	O3-C3-C4	2.19	115.26	110.34
2	Q	244	MMA	O5-C1-O1	2.37	116.58	110.88
2	O	240	MMA	O1-C1-C2	2.40	111.04	108.21
2	O	241	MAN	C1-C2-C3	2.41	112.39	109.54
2	P	242	MMA	O5-C5-C6	2.49	112.65	106.36
2	O	241	MAN	O3-C3-C4	2.57	116.13	110.34
2	O	240	MMA	C3-C4-C5	2.68	114.87	110.20
2	P	242	MMA	O5-C1-O1	3.27	118.75	110.88
2	P	242	MMA	O2-C2-C1	3.43	117.54	110.02
2	P	243	MAN	C1-O5-C5	3.45	116.62	112.25
2	Q	244	MMA	O2-C2-C1	3.56	117.82	110.02
2	R	246	MMA	O5-C5-C4	3.83	116.87	109.68
2	Q	245	MAN	C1-O5-C5	4.27	117.67	112.25
2	P	242	MMA	O1-C1-C2	8.90	118.71	108.21
2	Q	244	MMA	O1-C1-C2	9.98	119.98	108.21

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Q	244	MMA	C1
2	P	242	MMA	C1
2	R	246	MMA	C1
2	O	240	MMA	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	240	MMA	1	0
2	R	246	MMA	1	0
2	R	247	MAN	1	0

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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	234/237 (98%)	-0.38	2 (0%) 85 87	8, 14, 29, 46	6 (2%)
1	B	234/237 (98%)	-0.35	3 (1%) 79 82	9, 14, 28, 42	4 (1%)
1	C	234/237 (98%)	-0.12	5 (2%) 67 69	11, 20, 37, 45	6 (2%)
1	D	234/237 (98%)	-0.15	4 (1%) 73 75	9, 20, 36, 45	6 (2%)
All	All	936/948 (98%)	-0.25	14 (1%) 76 79	8, 17, 32, 46	22 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	SER	6.0
1	B	149	GLY	3.4
1	D	1	ALA	3.0
1	A	204	SER	2.9
1	D	205	HIS	2.7
1	D	204	SER	2.4
1	C	1	ALA	2.3
1	A	150	THR	2.3
1	B	150	THR	2.2
1	D	203	ASP	2.1
1	C	161	SER	2.0
1	C	150	THR	2.0
1	B	70	GLY	2.0
1	C	203	ASP	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](#)

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
2	MMA	O	240	13/13	0.88	0.30	5.39	42,53,59,60	0
2	MMA	R	246	13/13	0.75	0.36	4.53	40,52,58,59	0
2	MMA	Q	244	13/13	0.96	0.10	0.33	18,24,26,27	0
2	MAN	R	247	11/12	0.90	0.12	0.23	19,29,33,34	0
2	MAN	O	241	11/12	0.92	0.12	0.17	21,27,32,33	0
2	MAN	P	243	11/12	0.98	0.08	-0.10	8,13,15,16	0
2	MAN	Q	245	11/12	0.98	0.07	-0.31	9,14,16,18	0
2	MMA	P	242	13/13	0.96	0.09	-0.34	18,21,26,28	0

### 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	238	1/1	0.99	0.08	2.10	16,16,16,16	0
3	MN	A	238	1/1	0.99	0.08	1.54	16,16,16,16	0
4	CA	B	239	1/1	1.00	0.06	-1.44	11,11,11,11	0
4	CA	D	239	1/1	1.00	0.06	-1.73	17,17,17,17	0
4	CA	C	239	1/1	0.99	0.06	-2.05	17,17,17,17	0
3	MN	C	238	1/1	0.99	0.04	-3.18	21,21,21,21	0
3	MN	D	238	1/1	0.99	0.04	-3.29	21,21,21,21	0
4	CA	A	239	1/1	1.00	0.04	-4.61	12,12,12,12	0

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

There are no such residues in this entry.