



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 06:01 PM EDT

PDB ID : 7T84  
Title : Structure of angiotensin II type I receptor (AT1R) nanobody antagonist AT118i4h32 G26D T57I variant  
Authors : Nemeth, G.R.; Skiba, M.A.; Kruse, A.C.  
Deposited on : 2021-12-15  
Resolution : 1.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

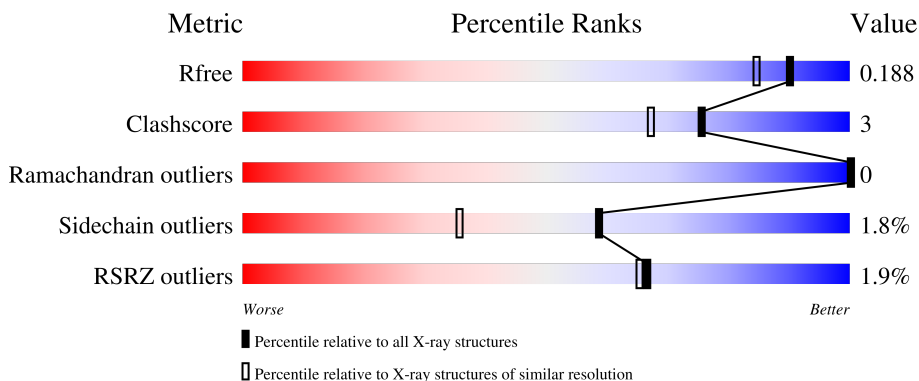
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	128	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      87%      6% • 6%</p>
1	B	128	<div style="display: flex; align-items: center;"> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">88%      6% • 5%</p>
1	C	128	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      88%      5% • 5%</p>
1	D	128	<div style="display: flex; align-items: center;"> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">87%      6% • 6%</p>
1	E	128	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      86%      5% • 8%</p>

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Mol	Chain	Length	Quality of chain
1	F	128	
1	G	128	
1	H	128	

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
3	GOL	B	202	-	X	-	-
5	PEG	F	201	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8637 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 Nanobody AT118i4h32 G26D T57I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	120	Total 946	C 587	N 171	O 183	S 5	0	3	0
1	B	121	Total 984	C 611	N 181	O 187	S 5	0	6	0
1	C	121	Total 955	C 595	N 172	O 183	S 5	0	3	0
1	D	120	Total 962	C 599	N 173	O 185	S 5	0	4	0
1	E	118	Total 980	C 612	N 176	O 187	S 5	0	9	0
1	F	117	Total 945	C 589	N 174	O 178	S 4	0	4	0
1	G	117	Total 956	C 595	N 175	O 182	S 4	0	6	0
1	H	116	Total 949	C 592	N 176	O 177	S 4	0	5	0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

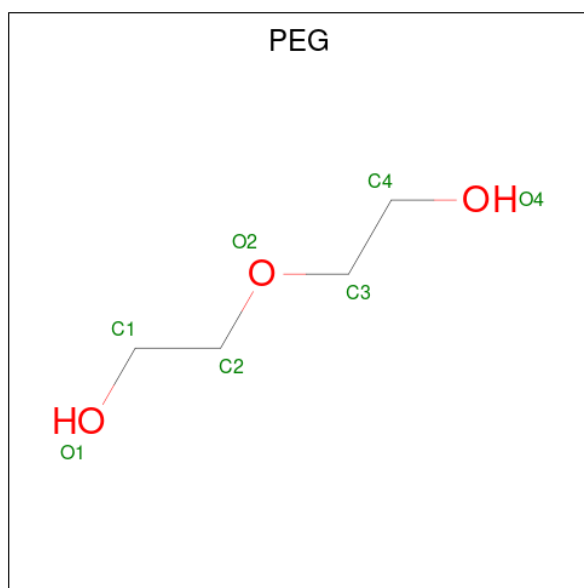


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			5	3	2		
5	D	1	Total	C	O	0	0
			5	3	2		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 5 3 2	0	0
5	F	1	Total C O 7 4 3	0	0
5	H	1	Total C O 7 4 3	0	0

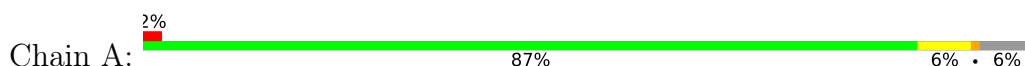
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	134	Total O 134 134	0	0
6	B	94	Total O 94 94	0	0
6	C	128	Total O 128 128	0	0
6	D	103	Total O 103 103	0	0
6	E	116	Total O 116 116	0	0
6	F	79	Total O 79 79	0	0
6	G	87	Total O 87 87	0	0
6	H	80	Total O 80 80	0	0

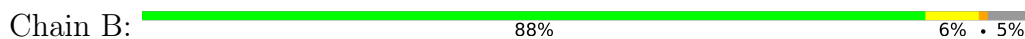
### 3 Residue-property plots [i](#)

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

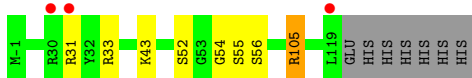
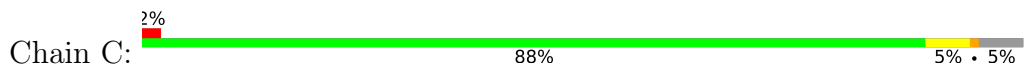
- Molecule 1: Nanobody AT118i4h32 G26D T57I



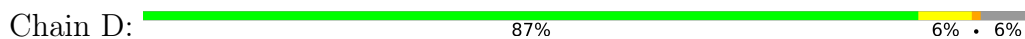
- Molecule 1: Nanobody AT118i4h32 G26D T57I



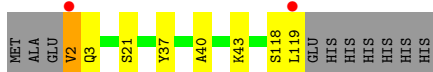
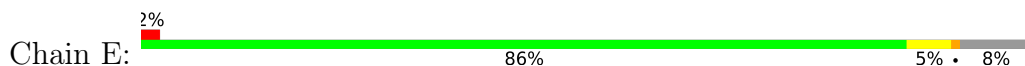
- Molecule 1: Nanobody AT118i4h32 G26D T57I



- Molecule 1: Nanobody AT118i4h32 G26D T57I

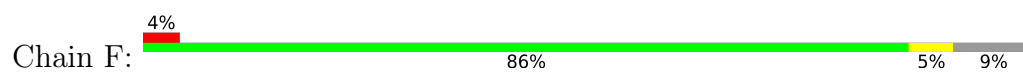


- Molecule 1: Nanobody AT118i4h32 G26D T57I

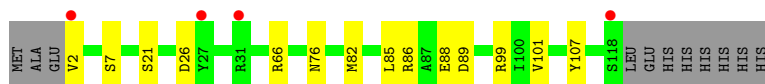
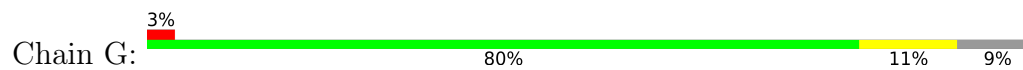


- Molecule 1: Nanobody AT118i4h32 G26D T57I

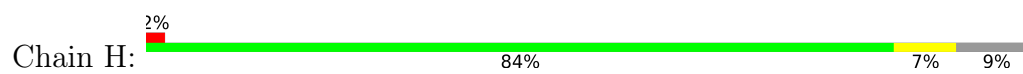




- Molecule 1: Nanobody AT118i4h32 G26D T57I



- Molecule 1: Nanobody AT118i4h32 G26D T57I



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.66Å 89.19Å 83.11Å 90.00° 110.05° 90.00°	Depositor
Resolution (Å)	46.32 – 1.60 46.32 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.32-1.60) 98.5 (46.32-1.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.60Å)	Xtrriage
Refinement program	PHENIX 1.19.2	Depositor
R, $R_{free}$	0.165 , 0.190 0.164 , 0.188	Depositor DCC
$R_{free}$ test set	1994 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, NA, CIT, PEG

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	0.55	0/964	0.72	0/1302
1	B	0.49	0/1002	0.72	0/1353
1	C	0.54	0/973	0.73	0/1315
1	D	0.48	0/982	0.71	0/1328
1	E	0.48	0/1000	0.72	0/1354
1	F	0.47	0/965	0.67	0/1305
1	G	0.43	0/976	0.70	0/1320
1	H	0.43	0/969	0.70	0/1310
All	All	0.49	0/7831	0.71	0/10587

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	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	C	105	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	105	ARG	Sidechain

## 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	946	0	915	8	0
1	B	984	0	960	3	0
1	C	955	0	930	7	0
1	D	962	0	924	8	0
1	E	980	0	944	5	0
1	F	945	0	910	4	0
1	G	956	0	919	10	0
1	H	949	0	918	6	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	E	26	0	10	0	0
2	H	13	0	5	0	0
3	B	6	0	7	1	0
3	C	12	0	15	0	0
3	E	6	0	8	1	0
4	B	1	0	0	0	0
5	C	12	0	15	3	0
5	D	18	0	22	4	0
5	E	5	0	5	2	0
5	F	7	0	10	2	0
5	H	7	0	10	0	0
6	A	134	0	0	1	0
6	B	94	0	0	0	0
6	C	128	0	0	1	0
6	D	103	0	0	1	0
6	E	116	0	0	0	0
6	F	79	0	0	0	0
6	G	87	0	0	2	0
6	H	80	0	0	1	0
All	All	8637	0	7537	48	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 3.

All (48) 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:G:99:ARG:NH1	6:G:201:HOH:O	2.20	0.74
1:G:66:ARG:NH2	1:G:89:ASP:OD2	2.22	0.73
1:C:52:SER:HA	5:C:204:PEG:H41	1.72	0.70
1:A:99:ARG:HH12	5:F:201:PEG:H11	1.63	0.61
1:A:30:ARG:NH1	6:A:301:HOH:O	2.34	0.60
1:D:105:ARG:HH22	5:D:203:PEG:H32	1.68	0.59
1:D:56[B]:SER:HB3	5:D:202:PEG:H12	1.84	0.59
1:G:82:MET:HE2	1:G:85:LEU:HD21	1.85	0.57
1:F:40:ALA:HB3	1:F:43:LYS:HE2	1.87	0.57
1:A:86:ARG:HH21	5:E:204:PEG:C2	2.19	0.56
1:C:56[B]:SER:OG	1:H:58:ASN:OD1	2.24	0.54
1:A:99:ARG:HH12	5:F:201:PEG:C1	2.21	0.52
1:F:36[B]:TRP:HZ3	1:F:78:VAL:HG12	1.75	0.52
1:D:56[A]:SER:HB2	5:D:202:PEG:H12	1.91	0.51
1:G:2:VAL:HG11	1:G:107:TYR:CD1	2.46	0.51
1:G:88:GLU:H	1:G:88:GLU:CD	2.14	0.50
1:B:31:ARG:HG3	1:B:32:TYR:CD1	2.47	0.50
1:G:7[B]:SER:OG	1:G:21:SER:OG	2.08	0.50
1:D:36[B]:TRP:CZ3	1:D:78:VAL:HG12	2.47	0.49
1:E:21:SER:HB3	5:E:204:PEG:H41	1.94	0.49
1:C:54:GLY:H	5:C:204:PEG:H42	1.79	0.48
1:G:26:ASP:OD1	1:G:76:ASN:ND2	2.44	0.47
1:A:30:ARG:HB2	1:A:31:ARG:NH1	2.30	0.47
1:G:7[A]:SER:HB3	1:G:21:SER:HG	1.80	0.47
1:C:54:GLY:H	5:C:204:PEG:C4	2.28	0.46
1:H:3:GLN:HB3	6:H:369:HOH:O	2.14	0.46
5:D:203:PEG:H21	5:D:203:PEG:H41	1.35	0.45
1:C:43:LYS:NZ	6:C:302:HOH:O	2.50	0.45
1:E:2:VAL:HB	1:E:3:GLN:H	1.54	0.45
1:E:37:TYR:HE2	3:E:203:GOL:H11	1.82	0.44
1:H:3:GLN:O	1:H:24:ALA:HA	2.17	0.44
1:A:27:TYR:HD1	1:A:31:ARG:HH21	1.64	0.44
2:A:201:CIT:O4	1:F:98:TYR:OH	2.25	0.44
1:D:62[B]:SER:OG	6:D:301:HOH:O	2.21	0.43
1:B:11:LEU:HD11	1:B:117:SER:HB3	2.01	0.43
1:C:105:ARG:NH2	1:D:105:ARG:NH2	2.67	0.43
1:D:12:VAL:HG11	1:D:85:LEU:HD13	2.01	0.42
1:G:101:VAL:HG13	6:G:239:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:SER:HB3	1:H:47:PHE:CD2	2.55	0.42
1:E:118[B]:SER:O	1:E:119:LEU:HB2	2.20	0.42
1:E:40:ALA:HB3	1:E:43:LYS:HD2	2.02	0.41
1:H:36[A]:TRP:HZ3	1:H:78[A]:VAL:HG12	1.85	0.41
1:H:18:LEU:HD12	1:H:114:VAL:HG13	2.02	0.41
1:A:105:ARG:NH2	1:B:105:ARG:NH2	2.68	0.41
1:D:36[B]:TRP:CZ3	1:D:80:LEU:HB2	2.56	0.41
1:G:66:ARG:NH2	1:G:86:ARG:HG3	2.36	0.41
1:A:108:TRP:O	3:B:202:GOL:O3	2.39	0.41
1:F:36[B]:TRP:CZ3	1:F:78:VAL:HG12	2.54	0.41

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	121/128 (94%)	115 (95%)	6 (5%)	0	100	100
1	B	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
1	C	122/128 (95%)	118 (97%)	4 (3%)	0	100	100
1	D	122/128 (95%)	117 (96%)	5 (4%)	0	100	100
1	E	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
1	F	119/128 (93%)	117 (98%)	2 (2%)	0	100	100
1	G	121/128 (94%)	118 (98%)	3 (2%)	0	100	100
1	H	119/128 (93%)	117 (98%)	2 (2%)	0	100	100
All	All	974/1024 (95%)	943 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	99/104 (95%)	97 (98%)	2 (2%)	55	31
1	B	103/104 (99%)	97 (94%)	6 (6%)	20	4
1	C	100/104 (96%)	98 (98%)	2 (2%)	55	31
1	D	100/104 (96%)	99 (99%)	1 (1%)	76	61
1	E	104/104 (100%)	103 (99%)	1 (1%)	76	61
1	F	98/104 (94%)	96 (98%)	2 (2%)	55	31
1	G	100/104 (96%)	100 (100%)	0	100	100
1	H	98/104 (94%)	97 (99%)	1 (1%)	76	61
All	All	802/832 (96%)	787 (98%)	15 (2%)	59	34

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	33	ARG
1	B	31	ARG
1	B	33	ARG
1	B	68[A]	THR
1	B	68[B]	THR
1	B	86	ARG
1	B	118	SER
1	C	31	ARG
1	C	33	ARG
1	D	33	ARG
1	E	2	VAL
1	F	19	ARG
1	F	26	ASP
1	H	26	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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
5	PEG	C	204	-	4,4,6	0.24	0	3,3,5	0.16	0
2	CIT	H	201	-	12,12,12	1.52	2 (16%)	17,17,17	2.14	9 (52%)
2	CIT	B	201	-	12,12,12	1.28	1 (8%)	17,17,17	2.21	6 (35%)
5	PEG	F	201	-	6,6,6	0.20	0	5,5,5	0.18	0
3	GOL	B	202	-	5,5,5	1.39	1 (20%)	5,5,5	1.69	2 (40%)
3	GOL	E	203	-	5,5,5	1.10	0	5,5,5	1.36	1 (20%)
5	PEG	E	204	-	4,4,6	0.15	0	3,3,5	0.23	0
2	CIT	E	201	-	12,12,12	1.12	0	17,17,17	1.27	2 (11%)
5	PEG	C	203	-	6,6,6	0.17	0	5,5,5	0.13	0
3	GOL	C	202	-	5,5,5	0.98	0	5,5,5	0.78	0
5	PEG	H	202	-	6,6,6	0.24	0	5,5,5	0.12	0
5	PEG	D	203	-	5,5,6	0.26	0	4,4,5	0.27	0
2	CIT	A	201	-	12,12,12	1.11	0	17,17,17	1.46	4 (23%)
2	CIT	E	202	-	12,12,12	1.04	0	17,17,17	1.40	1 (5%)
3	GOL	C	201	-	5,5,5	1.51	1 (20%)	5,5,5	1.20	0
5	PEG	D	201	-	4,4,6	0.23	0	3,3,5	0.22	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	D	202	-	6,6,6	0.15	0	5,5,5	0.19	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
5	PEG	C	204	-	-	2/2/2/4	-
2	CIT	H	201	-	-	3/16/16/16	-
2	CIT	B	201	-	-	3/16/16/16	-
5	PEG	F	201	-	-	2/4/4/4	-
3	GOL	B	202	-	-	4/4/4/4	-
3	GOL	E	203	-	-	0/4/4/4	-
5	PEG	E	204	-	-	1/2/2/4	-
2	CIT	E	201	-	-	0/16/16/16	-
5	PEG	C	203	-	-	2/4/4/4	-
3	GOL	C	202	-	-	2/4/4/4	-
5	PEG	H	202	-	-	4/4/4/4	-
5	PEG	D	203	-	-	3/3/3/4	-
2	CIT	A	201	-	-	2/16/16/16	-
2	CIT	E	202	-	-	2/16/16/16	-
3	GOL	C	201	-	-	2/4/4/4	-
5	PEG	D	201	-	-	1/2/2/4	-
5	PEG	D	202	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	CIT	C3-C6	2.63	1.56	1.53
3	B	202	GOL	O3-C3	-2.49	1.31	1.42
2	H	201	CIT	O5-C6	2.34	1.29	1.22
3	C	201	GOL	O1-C1	2.02	1.50	1.42
2	B	201	CIT	C2-C3	-2.01	1.51	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	CIT	O6-C6-C3	5.92	123.33	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	CIT	O7-C3-C2	-3.83	100.44	109.40
2	E	202	CIT	O6-C6-C3	3.54	119.20	113.05
2	B	201	CIT	O7-C3-C2	-3.30	101.68	109.40
2	E	201	CIT	O6-C6-C3	3.07	118.38	113.05
2	H	201	CIT	O5-C6-C3	2.97	126.46	122.25
2	A	201	CIT	O6-C6-C3	2.94	118.16	113.05
3	B	202	GOL	C3-C2-C1	-2.88	100.51	111.70
2	B	201	CIT	O7-C3-C6	2.78	112.77	108.86
2	H	201	CIT	C3-C4-C5	2.71	120.39	113.81
2	H	201	CIT	O1-C1-C2	-2.65	115.21	122.94
2	H	201	CIT	O4-C5-C4	2.58	122.63	114.35
2	H	201	CIT	O4-C5-O3	-2.53	116.98	123.30
2	B	201	CIT	C3-C2-C1	-2.52	107.71	113.81
2	H	201	CIT	O2-C1-C2	2.50	122.36	114.35
2	E	201	CIT	O5-C6-C3	-2.44	118.79	122.25
2	A	201	CIT	O4-C5-C4	2.44	122.17	114.35
3	E	203	GOL	C3-C2-C1	-2.37	102.50	111.70
2	B	201	CIT	O4-C5-O3	-2.19	117.84	123.30
3	B	202	GOL	O2-C2-C3	2.18	118.73	109.12
2	H	201	CIT	C4-C3-C2	2.17	114.82	109.16
2	H	201	CIT	O6-C6-O5	-2.14	117.00	123.82
2	B	201	CIT	O6-C6-O5	-2.07	117.22	123.82
2	A	201	CIT	O4-C5-O3	-2.04	118.20	123.30
2	A	201	CIT	O5-C6-C3	-2.02	119.39	122.25

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	GOL	O1-C1-C2-C3
3	B	202	GOL	C1-C2-C3-O3
5	D	203	PEG	C4-C3-O2-C2
5	C	204	PEG	O2-C3-C4-O4
2	B	201	CIT	C2-C3-C4-C5
2	B	201	CIT	C6-C3-C4-C5
3	C	201	GOL	O1-C1-C2-C3
3	C	202	GOL	O1-C1-C2-C3
3	B	202	GOL	O1-C1-C2-O2
3	B	202	GOL	O2-C2-C3-O3
3	C	202	GOL	O1-C1-C2-O2
5	C	203	PEG	O1-C1-C2-O2
5	F	201	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	C	201	GOL	O1-C1-C2-O2
2	B	201	CIT	O7-C3-C4-C5
5	D	203	PEG	C1-C2-O2-C3
5	E	204	PEG	C4-C3-O2-C2
5	H	202	PEG	O1-C1-C2-O2
2	H	201	CIT	C6-C3-C4-C5
5	C	204	PEG	C4-C3-O2-C2
5	H	202	PEG	C1-C2-O2-C3
5	D	202	PEG	C1-C2-O2-C3
5	D	201	PEG	C4-C3-O2-C2
5	C	203	PEG	C1-C2-O2-C3
2	H	201	CIT	O7-C3-C4-C5
2	A	201	CIT	C2-C3-C6-O5
5	D	202	PEG	O1-C1-C2-O2
2	H	201	CIT	C2-C3-C4-C5
5	H	202	PEG	O2-C3-C4-O4
5	D	203	PEG	O2-C3-C4-O4
5	H	202	PEG	C4-C3-O2-C2
2	A	201	CIT	C2-C3-C6-O6
5	F	201	PEG	C1-C2-O2-C3
2	E	202	CIT	O1-C1-C2-C3
2	E	202	CIT	O2-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	204	PEG	3	0
5	F	201	PEG	2	0
3	B	202	GOL	1	0
3	E	203	GOL	1	0
5	E	204	PEG	2	0
5	D	203	PEG	2	0
2	A	201	CIT	1	0
5	D	202	PEG	2	0

## 5.7 Other polymers [i](#)

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	120/128 (93%)	-0.29	2 (1%) 70 69	16, 23, 37, 54	0
1	B	121/128 (94%)	-0.17	0 100 100	18, 30, 49, 74	0
1	C	121/128 (94%)	-0.15	3 (2%) 57 55	16, 23, 39, 64	0
1	D	120/128 (93%)	-0.37	0 100 100	18, 28, 45, 68	0
1	E	118/128 (92%)	-0.11	2 (1%) 70 69	18, 27, 50, 65	0
1	F	117/128 (91%)	-0.00	5 (4%) 35 32	22, 34, 58, 74	0
1	G	117/128 (91%)	-0.03	4 (3%) 45 42	23, 32, 59, 80	0
1	H	116/128 (90%)	-0.17	2 (1%) 70 69	23, 34, 58, 74	0
All	All	950/1024 (92%)	-0.16	18 (1%) 66 65	16, 29, 55, 80	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	VAL	7.8
1	E	2	VAL	5.5
1	G	2	VAL	4.4
1	G	27	TYR	3.1
1	H	42	GLY	3.0
1	F	118	SER	3.0
1	F	42	GLY	2.7
1	G	118	SER	2.7
1	E	119	LEU	2.6
1	A	31	ARG	2.6
1	F	41	PRO	2.6
1	C	30	ARG	2.5
1	C	119	LEU	2.5
1	A	30	ARG	2.4
1	F	14	PRO	2.3
1	G	31	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	ARG	2.2
1	H	30	ARG	2.1

## 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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	PEG	D	203	6/7	0.70	0.24	43,50,60,64	0
5	PEG	D	201	5/7	0.75	0.24	43,45,55,58	0
5	PEG	F	201	7/7	0.75	0.43	43,44,47,47	0
5	PEG	C	203	7/7	0.76	0.27	35,52,59,62	0
2	CIT	B	201	13/13	0.79	0.18	30,40,45,50	0
5	PEG	E	204	5/7	0.80	0.21	36,42,49,51	0
5	PEG	C	204	5/7	0.83	0.28	33,37,48,52	0
2	CIT	H	201	13/13	0.84	0.15	29,40,46,49	0
2	CIT	E	202	13/13	0.85	0.16	32,46,58,61	0
5	PEG	D	202	7/7	0.87	0.24	40,40,48,55	0
3	GOL	E	203	6/6	0.87	0.16	29,33,36,48	0
3	GOL	C	202	6/6	0.89	0.22	32,38,40,48	0
5	PEG	H	202	7/7	0.89	0.24	29,42,52,57	0
2	CIT	A	201	13/13	0.90	0.11	26,36,44,46	0
2	CIT	E	201	13/13	0.91	0.12	25,33,40,42	0
3	GOL	B	202	6/6	0.92	0.13	25,30,34,38	0
3	GOL	C	201	6/6	0.95	0.09	23,32,35,40	0
4	NA	B	203	1/1	0.99	0.07	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.