Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:04 PM GMT

PDB ID	:	5AWV
Title	:	Crystal structure of glycopeptide hexose oxidase DBV29 complexed with teicoplanin
Authors	:	Liu, Y.C.; Li, T.L.
Deposited on	:	2015-07-09
Resolution	:	1.93 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

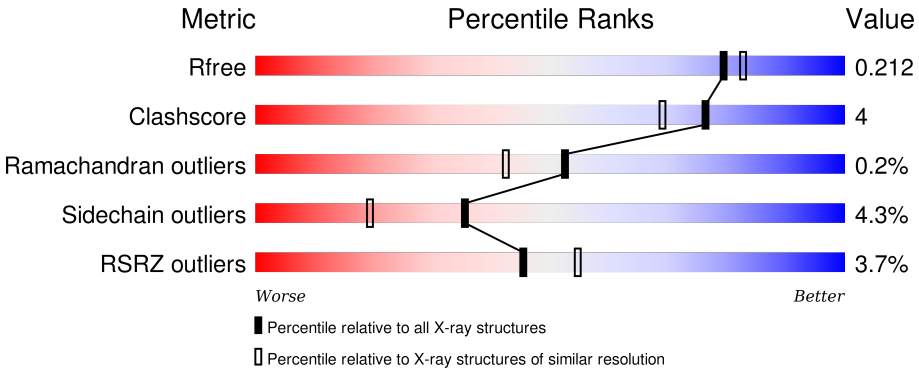
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.93 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 >=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 <=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	523	2% 84% 10% • 5%
1	B	523	2% 84% 10% • 5%
1	C	523	4% 85% 9% • 5%
1	D	523	7% 85% 10% • 5%
2	I	7	71% 29%

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Mol	Chain	Length	Quality of chain
2	J	7	100%
2	K	7	86% 14%
2	L	7	43% 57%
2	M	7	86% 14%
2	N	7	86% 14%
2	O	7	100%
2	P	7	100%

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
4	CIT	A	602	-	-	-	X
4	CIT	B	603	-	-	-	X
4	CIT	C	602	-	-	-	X
4	CIT	D	602	-	-	-	X
5	T55	B	602	-	-	-	X
5	T55	K	101	-	-	-	X
5	T55	M	101	-	-	-	X
5	T55	N	101	-	-	X	X
5	T55	P	101	-	-	-	X
6	MAN	P	102	-	-	-	X
7	NAG	K	103	-	-	-	X
7	NAG	L	102	-	-	-	X
7	NAG	M	103	-	-	-	X
8	N1L	K	104	-	-	-	X
8	N1L	L	103	-	-	-	X
8	N1L	M	104	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18119 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.

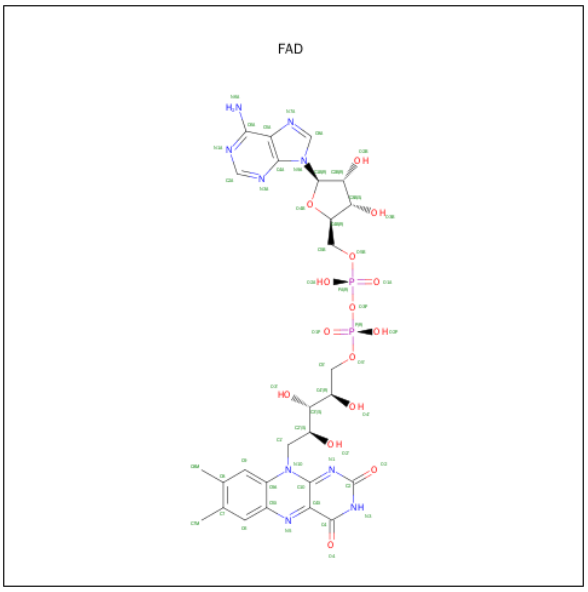
- Molecule 1 is a protein called Putative hexose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			
1	B	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			
1	C	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			
1	D	498	Total	C	N	O	S	0	0	0
			3856	2441	685	716	14			

- Molecule 2 is a protein called TEICOPLANIN.

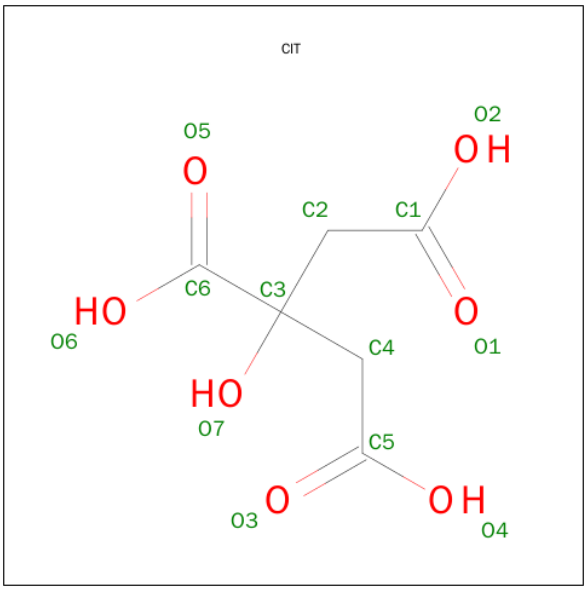
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	J	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	K	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	L	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	M	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	N	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	O	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	P	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



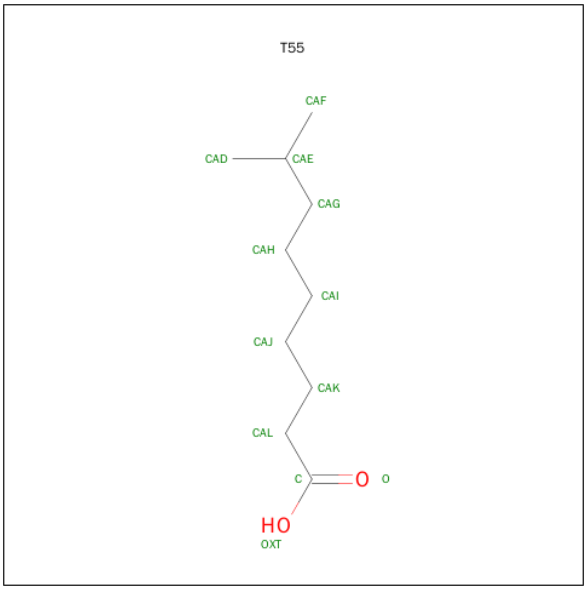
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



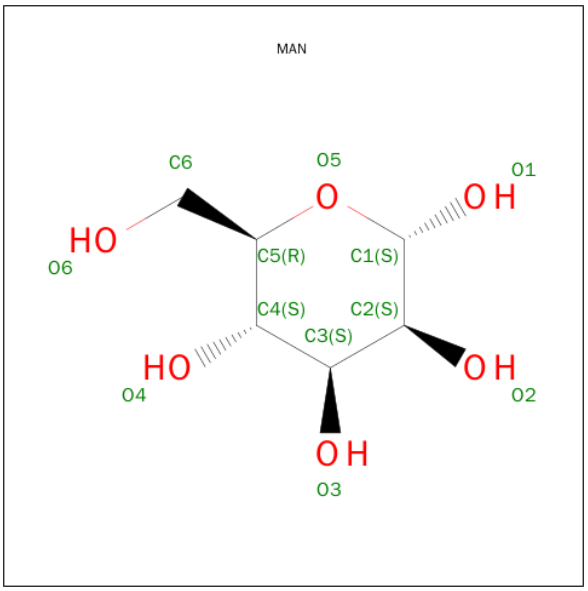
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0
4	O	1	Total C O 13 6 7	0	0

- Molecule 5 is 8-METHYLNONANOIC ACID (three-letter code: T55) (formula: $C_{10}H_{20}O_2$).



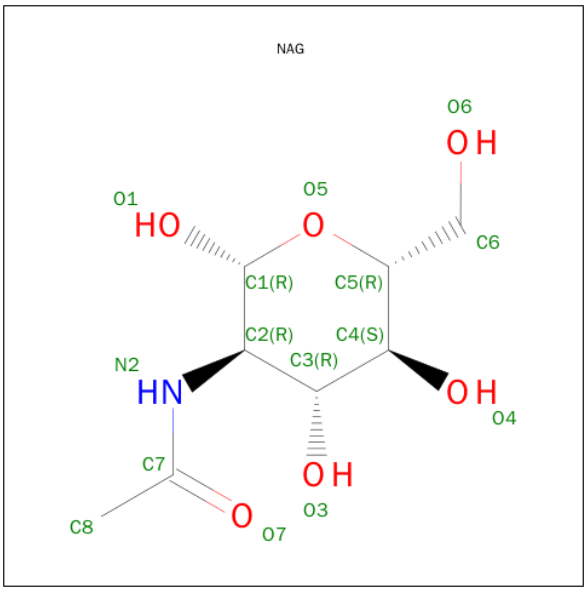
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 11 10 1	0	0
5	K	1	Total C O 11 10 1	0	0
5	M	1	Total C O 11 10 1	0	0
5	N	1	Total C O 11 10 1	0	0
5	O	1	Total C O 11 10 1	0	0
5	P	1	Total C O 11 10 1	0	0

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



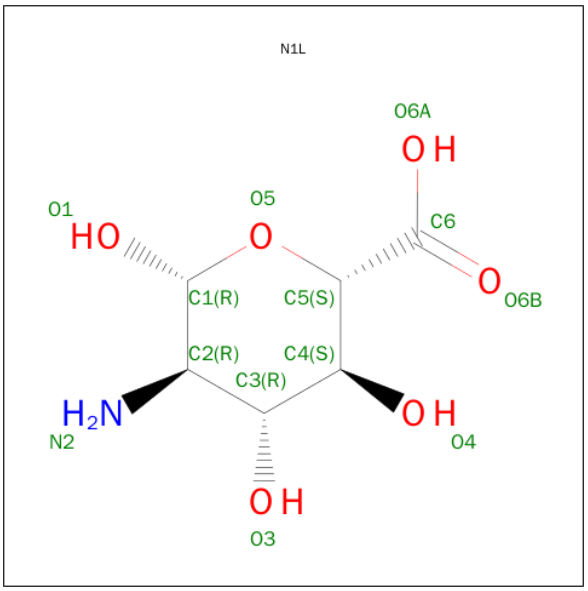
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 11 6 5	0	0
6	J	1	Total C O 11 6 5	0	0
6	K	1	Total C O 11 6 5	0	0
6	L	1	Total C O 11 6 5	0	0
6	M	1	Total C O 11 6 5	0	0
6	N	1	Total C O 11 6 5	0	0
6	O	1	Total C O 11 6 5	0	0
6	P	1	Total C O 11 6 5	0	0

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C N O 14 8 1 5	0	0
7	J	1	Total C N O 14 8 1 5	0	0
7	K	1	Total C N O 14 8 1 5	0	0
7	L	1	Total C N O 14 8 1 5	0	0
7	M	1	Total C N O 14 8 1 5	0	0
7	N	1	Total C N O 14 8 1 5	0	0
7	O	1	Total C N O 14 8 1 5	0	0
7	P	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is 2-AMINO-2-DEOXY-BETA-D-GLUCOPYRANURONIC ACID (three-letter code: N1L) (formula: $C_6H_{11}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	1	Total C N O 12 6 1 5	0	0
8	L	1	Total C N O 12 6 1 5	0	0
8	M	1	Total C N O 12 6 1 5	0	0
8	N	1	Total C N O 12 6 1 5	0	0
8	O	1	Total C N O 12 6 1 5	0	0
8	P	1	Total C N O 12 6 1 5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	425	Total O 425 425	0	0
9	B	379	Total O 379 379	0	0
9	C	327	Total O 327 327	0	0
9	D	217	Total O 217 217	0	0
9	I	6	Total O 6 6	0	0
9	J	5	Total O 5 5	0	0

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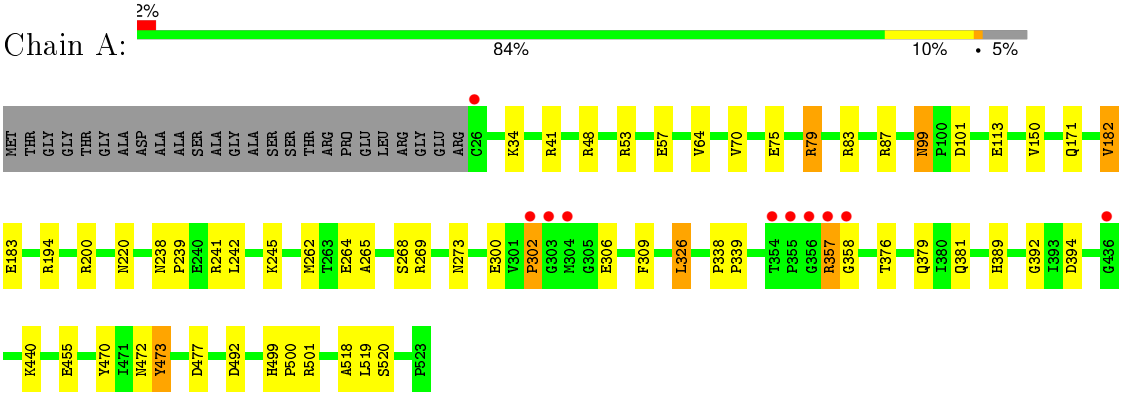
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	K	3	Total O 3 3	0	0
9	L	1	Total O 1 1	0	0
9	M	1	Total O 1 1	0	0
9	N	12	Total O 12 12	0	0
9	O	16	Total O 16 16	0	0
9	P	8	Total O 8 8	0	0

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 (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.

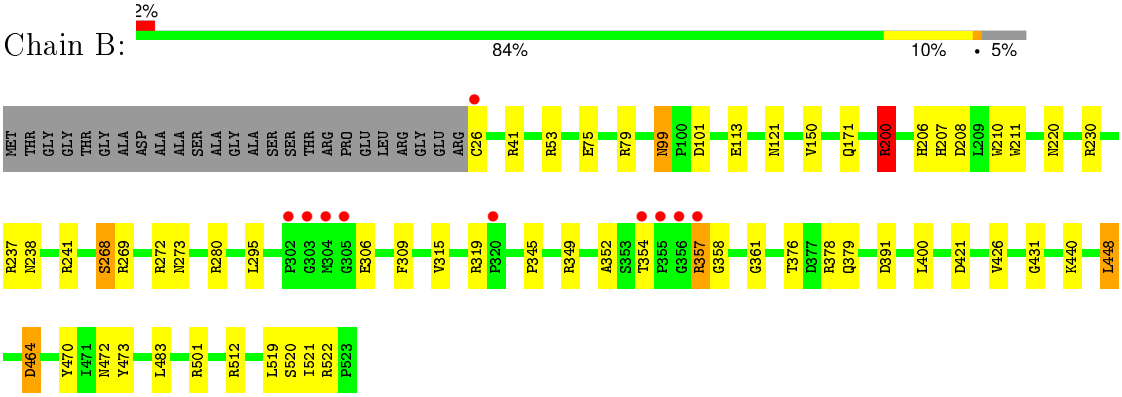
- Molecule 1: Putative hexose oxidase

Chain A:



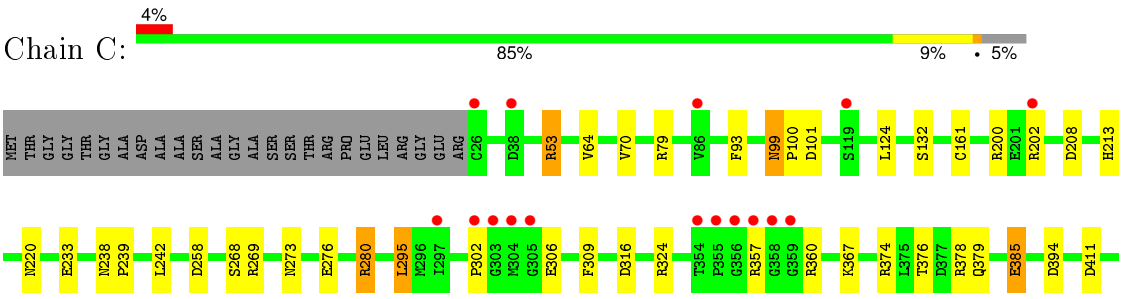
- Molecule 1: Putative hexose oxidase

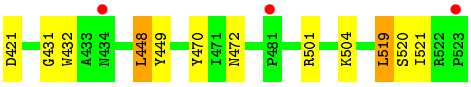
Chain B:



- Molecule 1: Putative hexose oxidase

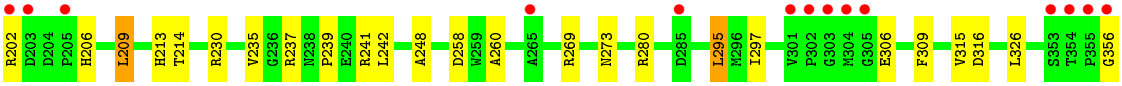
Chain C:

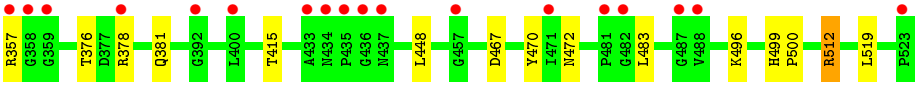




• Molecule 1: Putative hexose oxidase

Chain D:



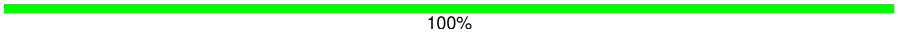


• Molecule 2: TEICOPLANIN

Chain I:

• Molecule 2: TEICOPLANIN

Chain J:



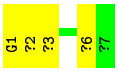
There are no outlier residues recorded for this chain.

• Molecule 2: TEICOPLANIN

Chain K:

• Molecule 2: TEICOPLANIN

Chain L:

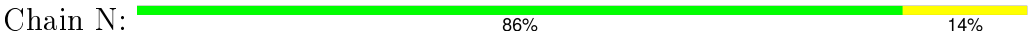


• Molecule 2: TEICOPLANIN

Chain M:

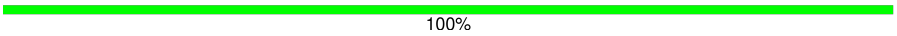
• Molecule 2: TEICOPLANIN

Chain N:



- Molecule 2: TEICOPLANIN

Chain O:



There are no outlier residues recorded for this chain.

- Molecule 2: TEICOPLANIN

Chain P:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.79Å 150.78Å 124.85Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	29.40 – 1.93 29.49 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.40-1.93) 97.6 (29.49-1.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.156 , 0.205 0.167 , 0.212	Depositor DCC
R_{free} test set	8214 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 163844 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18119	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GHP, NAG, 3MY, T55, N1L, CIT, 3FG, OMY, FAD, 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	1.07	3/3966 (0.1%)	1.04	16/5412 (0.3%)
1	B	1.02	1/3966 (0.0%)	1.03	14/5412 (0.3%)
1	C	0.95	0/3966	1.02	16/5412 (0.3%)
1	D	0.85	0/3966	0.94	9/5412 (0.2%)
All	All	0.98	4/15864 (0.0%)	1.01	55/21648 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	GLU	CD-OE1	7.79	1.34	1.25
1	A	53	ARG	CZ-NH1	5.67	1.40	1.33
1	A	183	GLU	CD-OE2	-5.50	1.19	1.25
1	A	264	GLU	CD-OE2	5.15	1.31	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	53	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	53	ARG	NE-CZ-NH2	-10.15	115.23	120.30
1	B	53	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	C	53	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	C	448	LEU	CB-CG-CD2	8.79	125.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	316	ASP	CB-CG-OD1	8.36	125.83	118.30
1	A	41	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	512	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	53	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	200	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	B	448	LEU	CB-CG-CD2	7.79	124.24	111.00
1	D	87	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	200	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	374	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	421	ASP	CB-CG-OD1	7.24	124.81	118.30
1	C	324	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	391	ASP	CB-CG-OD1	6.96	124.57	118.30
1	D	87	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	477	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	53	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	200	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	421	ASP	CB-CG-OD1	6.59	124.24	118.30
1	B	391	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	512	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	200	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	230	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	41	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	280	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	326	LEU	CB-CG-CD2	5.92	121.07	111.00
1	D	53	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	87	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	48	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	241	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	280	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	501	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	200	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	D	202	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	519	LEU	CB-CG-CD1	5.48	120.32	111.00
1	D	316	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	492	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	501	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	378	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	208	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	87	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	182	VAL	CB-CA-C	-5.30	101.33	111.40
1	A	473	TYR	CB-CG-CD2	-5.30	117.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	448	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	83	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	41	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	295	LEU	CB-CG-CD2	5.17	119.79	111.00
1	C	501	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	D	79	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	138	LEU	CB-CG-CD1	5.06	119.60	111.00
1	D	170	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	357	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3743	38	0
1	B	3856	0	3743	29	0
1	C	3856	0	3744	27	0
1	D	3856	0	3744	21	0
2	I	85	0	35	2	0
2	J	85	0	36	0	0
2	K	85	0	32	1	0
2	L	85	0	34	3	0
2	M	85	0	34	1	0
2	N	85	0	34	5	0
2	O	85	0	36	0	0
2	P	85	0	34	0	0
3	A	53	0	29	0	0
3	B	53	0	29	0	0
3	C	53	0	29	0	0
3	D	53	0	29	0	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	13	0	5	0	0
4	D	13	0	5	0	0
4	O	13	0	5	0	0
5	B	11	0	19	1	0
5	K	11	0	19	1	0
5	M	11	0	19	4	0
5	N	11	0	19	14	0
5	O	11	0	19	0	0
5	P	11	0	19	0	1
6	I	11	0	10	0	0
6	J	11	0	10	0	0
6	K	11	0	10	0	0
6	L	11	0	10	0	0
6	M	11	0	10	0	0
6	N	11	0	10	0	0
6	O	11	0	9	0	0
6	P	11	0	10	0	0
7	I	14	0	13	0	0
7	J	14	0	13	0	0
7	K	14	0	13	0	0
7	L	14	0	13	3	0
7	M	14	0	13	0	0
7	N	14	0	13	0	0
7	O	14	0	13	0	0
7	P	14	0	13	0	0
8	K	12	0	7	1	0
8	L	12	0	7	2	0
8	M	12	0	7	1	0
8	N	12	0	6	0	0
8	O	12	0	7	0	0
8	P	12	0	6	0	0
9	A	425	0	0	10	4
9	B	379	0	0	7	1
9	C	327	0	0	7	1
9	D	217	0	0	5	0
9	I	6	0	0	0	0
9	J	5	0	0	0	0
9	K	3	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
9	N	12	0	0	0	0
9	O	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	8	0	0	0	0
All	All	18119	0	15727	123	4

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 4.

All (123) 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:A:265:ALA:HA	5:N:101:T55:CAD	1.84	1.06
1:A:265:ALA:HA	5:N:101:T55:HAD1	1.51	0.92
1:D:269:ARG:HE	1:D:273:ASN:HD21	1.23	0.86
1:C:269:ARG:HE	1:C:273:ASN:HD21	1.23	0.86
1:A:519:LEU:N	9:A:701:HOH:O	1.59	0.81
1:C:93:PHE:CZ	8:M:104:N1L:O4	2.33	0.80
1:D:512:ARG:NH1	9:D:701:HOH:O	2.14	0.79
1:C:411:ASP:OD1	9:C:701:HOH:O	2.03	0.76
1:A:265:ALA:HA	5:N:101:T55:HAD2	1.65	0.76
1:A:265:ALA:CA	5:N:101:T55:HAD2	2.17	0.75
1:A:265:ALA:CA	5:N:101:T55:CAD	2.65	0.75
1:B:400:LEU:HD23	1:B:426:VAL:HG22	1.71	0.73
1:A:376:THR:H	1:A:379:GLN:HE21	1.37	0.72
1:B:519:LEU:N	9:B:701:HOH:O	1.62	0.71
1:A:57:GLU:OE1	9:A:702:HOH:O	2.09	0.69
1:C:208:ASP:HB2	9:C:731:HOH:O	1.92	0.69
2:N:2:3MY:HB2C	5:N:101:T55:HAG1	1.75	0.68
1:B:376:THR:H	1:B:379:GLN:HE21	1.42	0.67
1:C:376:THR:H	1:C:379:GLN:HE21	1.40	0.67
1:A:265:ALA:CB	5:N:101:T55:HAD2	2.26	0.66
2:N:2:3MY:OBD	5:N:101:T55:O	2.13	0.66
1:B:280:ARG:HD2	9:B:993:HOH:O	1.97	0.65
1:C:269:ARG:HE	1:C:273:ASN:ND2	1.96	0.63
1:B:361:GLY:HA2	7:L:102:NAG:H3	1.80	0.62
1:C:233:GLU:OE2	9:C:702:HOH:O	2.16	0.62
1:A:381:GLN:HG2	9:O:206:HOH:O	2.00	0.61
1:A:171:GLN:HG3	9:A:889:HOH:O	2.01	0.60
1:A:99:ASN:HD22	1:A:101:ASP:H	1.49	0.60
1:A:470:TYR:CZ	1:A:472:ASN:HB2	2.36	0.60
1:A:220:ASN:HD21	1:A:520:SER:HA	1.67	0.59
1:D:57:GLU:HG3	9:D:716:HOH:O	2.03	0.59
1:A:518:ALA:CA	9:A:701:HOH:O	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:GLU:O	1:C:280:ARG:HD3	2.02	0.58
1:A:455:GLU:OE1	9:A:703:HOH:O	2.17	0.58
1:C:239:PRO:HA	1:C:242:LEU:HD12	1.84	0.58
1:B:269:ARG:HE	1:B:273:ASN:HD21	1.51	0.58
1:B:473:TYR:CZ	8:L:103:N1L:O6B	2.57	0.57
1:B:470:TYR:CZ	1:B:472:ASN:HB2	2.40	0.57
1:A:518:ALA:N	9:A:701:HOH:O	2.39	0.55
1:D:121:ASN:HD21	1:D:237:ARG:HA	1.71	0.55
1:D:188:ASN:O	1:D:512:ARG:HD2	2.08	0.54
1:A:389:HIS:CE1	9:A:887:HOH:O	2.60	0.54
1:C:504:LYS:HD2	9:C:703:HOH:O	2.08	0.54
1:B:99:ASN:HD22	1:B:101:ASP:H	1.56	0.54
1:A:150:VAL:HB	2:K:2:3MY:CL	2.45	0.54
1:D:470:TYR:CZ	1:D:472:ASN:HB2	2.43	0.54
1:C:470:TYR:CZ	1:C:472:ASN:HB2	2.43	0.53
1:D:280:ARG:NH1	9:D:707:HOH:O	2.42	0.52
1:B:473:TYR:OH	8:L:103:N1L:O6B	2.23	0.52
1:A:357:ARG:HG3	1:A:358:GLY:HA3	1.91	0.52
1:B:522:ARG:O	9:B:702:HOH:O	2.19	0.51
1:B:268:SER:OG	1:B:272:ARG:NH1	2.44	0.51
1:A:357:ARG:HG2	9:A:916:HOH:O	2.10	0.51
1:D:295:LEU:HD13	1:D:297:ILE:HD11	1.93	0.51
1:D:99:ASN:HD22	1:D:101:ASP:H	1.59	0.50
1:A:241:ARG:NH1	9:A:707:HOH:O	2.44	0.50
1:A:269:ARG:HE	1:A:273:ASN:HD21	1.60	0.50
1:B:200:ARG:HB3	1:B:210:TRP:CE2	2.46	0.50
1:C:208:ASP:OD2	9:C:703:HOH:O	2.20	0.48
1:B:171:GLN:HG3	9:B:884:HOH:O	2.12	0.48
2:N:2:3MY:CB	5:N:101:T55:HAG1	2.43	0.48
1:D:258:ASP:OD2	1:D:260:ALA:HB3	2.13	0.48
1:B:207:HIS:CE1	2:I:3:3FG:HG1	2.49	0.48
1:B:431:GLY:C	5:B:602:T55:HAD2	2.33	0.48
1:C:394:ASP:HB2	5:M:101:T55:HAD1	1.94	0.48
1:B:220:ASN:HD21	1:B:520:SER:HA	1.79	0.48
1:A:392:GLY:HA3	1:A:440:LYS:HE2	1.97	0.47
1:C:64:VAL:HG21	1:C:70:VAL:HG22	1.97	0.47
1:D:235:VAL:O	1:D:235:VAL:HG12	2.14	0.47
1:A:262:MET:CE	1:A:339:PRO:HG2	2.45	0.47
1:A:245:LYS:HE2	1:A:245:LYS:HB2	1.83	0.46
1:C:220:ASN:HD21	1:C:520:SER:HA	1.81	0.46
1:B:357:ARG:NH2	2:L:6:OMY:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:CZ	8:K:104:N1L:O6B	2.68	0.46
1:C:53:ARG:NH2	9:C:706:HOH:O	2.42	0.46
1:A:265:ALA:CA	5:N:101:T55:HAD1	2.36	0.45
1:A:239:PRO:HA	1:A:242:LEU:HD12	1.97	0.45
1:C:431:GLY:C	5:M:101:T55:HAD2	2.37	0.45
1:C:99:ASN:HD22	1:C:101:ASP:H	1.63	0.45
2:M:6:OMY:CL	5:M:101:T55:O	2.72	0.45
1:B:349:ARG:HB2	1:B:352:ALA:HB2	1.99	0.45
1:B:464:ASP:HB2	9:B:933:HOH:O	2.16	0.45
1:D:214:THR:HB	1:D:415:THR:HB	1.98	0.45
1:D:248:ALA:HA	9:D:871:HOH:O	2.17	0.45
1:B:79:ARG:HD2	9:B:1052:HOH:O	2.17	0.45
1:B:358:GLY:C	7:L:102:NAG:H81	2.37	0.45
1:A:99:ASN:HD22	1:A:101:ASP:N	2.14	0.45
1:B:357:ARG:NH2	7:L:102:NAG:H83	2.31	0.44
1:A:268:SER:HB3	5:N:101:T55:HAD3	1.98	0.44
1:D:499:HIS:HB3	1:D:500:PRO:HD3	2.00	0.44
1:B:206:HIS:HD2	9:B:742:HOH:O	2.00	0.44
1:B:400:LEU:HD23	1:B:426:VAL:CG2	2.45	0.44
1:B:220:ASN:ND2	1:B:521:ILE:H	2.16	0.44
2:L:1:GHP:C2	2:L:3:3FG:CG2	2.94	0.43
1:A:79:ARG:NE	9:A:714:HOH:O	2.51	0.43
1:A:394:ASP:HB3	5:K:101:T55:HAD1	2.00	0.43
1:B:150:VAL:HB	2:L:2:3MY:CL	2.56	0.43
1:D:239:PRO:HA	1:D:242:LEU:HD12	2.00	0.43
1:C:269:ARG:NE	1:C:273:ASN:HD21	2.03	0.42
2:I:1:GHP:C2	2:I:3:3FG:HG2	2.49	0.42
1:D:64:VAL:HG21	1:D:70:VAL:HG22	2.00	0.42
1:C:394:ASP:CB	5:M:101:T55:HAD1	2.49	0.42
1:D:188:ASN:OD1	1:D:188:ASN:C	2.58	0.42
1:D:209:LEU:HD22	1:D:213:HIS:CE1	2.54	0.42
2:N:2:3MY:CZ	5:N:101:T55:HAK1	2.50	0.42
2:N:2:3MY:CG	5:N:101:T55:HAI1	2.50	0.42
1:C:53:ARG:HD2	1:C:432:TRP:CZ2	2.54	0.41
1:D:99:ASN:HD21	1:D:101:ASP:HB2	1.85	0.41
1:A:338:PRO:N	1:A:339:PRO:CD	2.84	0.41
1:C:385:GLU:HG2	9:C:954:HOH:O	2.18	0.41
1:B:121:ASN:HD21	1:B:237:ARG:HA	1.86	0.41
1:C:161:CYS:HA	1:C:213:HIS:O	2.20	0.41
1:C:99:ASN:HB2	1:C:100:PRO:HD2	2.01	0.41
1:A:64:VAL:HG21	1:A:70:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ASP:OD1	1:D:496:LYS:NZ	2.36	0.40
1:B:211:TRP:CZ3	1:B:501:ARG:HG2	2.56	0.40
1:C:367:LYS:HE3	1:C:449:TYR:CD2	2.56	0.40
1:A:265:ALA:HB1	5:N:101:T55:HAD2	1.99	0.40
1:C:53:ARG:HD2	1:C:432:TRP:HZ2	1.87	0.40
1:C:220:ASN:ND2	1:C:521:ILE:H	2.19	0.40
1:A:499:HIS:N	1:A:500:PRO:CD	2.85	0.40
1:A:499:HIS:HB3	1:A:500:PRO:HD3	2.02	0.40
1:D:206:HIS:HD2	9:D:727:HOH:O	2.04	0.40

All (4) 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)
9:A:800:HOH:O	9:C:948:HOH:O[1_655]	2.02	0.18
9:A:722:HOH:O	9:A:890:HOH:O[1_455]	2.02	0.18
5:P:101:T55:CAD	9:A:724:HOH:O[2_7413]	2.16	0.04
9:A:886:HOH:O	9:B:983:HOH:O[2_7513]	2.19	0.01

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	496/523 (95%)	479 (97%)	16 (3%)	1 (0%)	52 42
1	B	496/523 (95%)	478 (96%)	18 (4%)	0	100 100
1	C	496/523 (95%)	478 (96%)	17 (3%)	1 (0%)	52 42
1	D	496/523 (95%)	473 (95%)	21 (4%)	2 (0%)	39 26
All	All	1984/2092 (95%)	1908 (96%)	72 (4%)	4 (0%)	52 42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	PRO
1	D	356	GLY
1	D	376	THR
1	C	302	PRO

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	404/419 (96%)	390 (96%)	14 (4%)	43	28
1	B	404/419 (96%)	386 (96%)	18 (4%)	34	18
1	C	404/419 (96%)	387 (96%)	17 (4%)	36	20
1	D	404/419 (96%)	383 (95%)	21 (5%)	29	13
All	All	1616/1676 (96%)	1546 (96%)	70 (4%)	35	19

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	75	GLU
1	A	79	ARG
1	A	99	ASN
1	A	113	GLU
1	A	182	VAL
1	A	194	ARG
1	A	238	ASN
1	A	300	GLU
1	A	302	PRO
1	A	306	GLU
1	A	309	PHE
1	A	326	LEU
1	A	357	ARG
1	B	26	CYS
1	B	99	ASN
1	B	113	GLU
1	B	200	ARG

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Mol	Chain	Res	Type
1	B	238	ASN
1	B	268	SER
1	B	295	LEU
1	B	306	GLU
1	B	309	PHE
1	B	315	VAL
1	B	319	ARG
1	B	345	PRO
1	B	354	THR
1	B	357	ARG
1	B	440	LYS
1	B	448	LEU
1	B	464	ASP
1	B	483	LEU
1	C	79	ARG
1	C	99	ASN
1	C	124	LEU
1	C	132	SER
1	C	202	ARG
1	C	238	ASN
1	C	258	ASP
1	C	268	SER
1	C	295	LEU
1	C	306	GLU
1	C	309	PHE
1	C	357	ARG
1	C	360	ARG
1	C	378	ARG
1	C	385	GLU
1	C	448	LEU
1	C	519	LEU
1	D	45	LEU
1	D	99	ASN
1	D	121	ASN
1	D	124	LEU
1	D	138	LEU
1	D	182	VAL
1	D	194	ARG
1	D	209	LEU
1	D	230	ARG
1	D	241	ARG
1	D	295	LEU

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Mol	Chain	Res	Type
1	D	306	GLU
1	D	309	PHE
1	D	315	VAL
1	D	326	LEU
1	D	378	ARG
1	D	381	GLN
1	D	448	LEU
1	D	483	LEU
1	D	512	ARG
1	D	519	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	99	ASN
1	A	121	ASN
1	A	207	HIS
1	A	220	ASN
1	A	238	ASN
1	A	273	ASN
1	A	348	GLN
1	A	379	GLN
1	A	437	ASN
1	A	513	ASN
1	B	99	ASN
1	B	121	ASN
1	B	207	HIS
1	B	220	ASN
1	B	238	ASN
1	B	273	ASN
1	B	379	GLN
1	B	437	ASN
1	B	513	ASN
1	C	55	ASN
1	C	99	ASN
1	C	121	ASN
1	C	220	ASN
1	C	238	ASN
1	C	273	ASN
1	C	379	GLN
1	C	513	ASN

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Mol	Chain	Res	Type
1	D	55	ASN
1	D	99	ASN
1	D	121	ASN
1	D	190	GLN
1	D	207	HIS
1	D	220	ASN
1	D	273	ASN
1	D	348	GLN
1	D	379	GLN
1	D	381	GLN
1	D	513	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

56 non-standard protein/DNA/RNA residues 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	GHP	I	1	2	10,11,12	2.83	1 (10%)	12,14,16	0.98	0
2	3MY	I	2	2	11,13,14	2.23	3 (27%)	15,17,19	1.98	3 (20%)
2	3FG	I	3	2	11,12,13	2.97	2 (18%)	14,16,18	2.29	5 (35%)
2	GHP	I	4	2	10,11,12	2.40	3 (30%)	12,14,16	1.14	0
2	GHP	I	5	2	10,11,12	2.91	2 (20%)	12,14,16	2.11	3 (25%)
2	OMY	I	6	2,7	13,14,15	2.75	7 (53%)	16,19,21	1.66	3 (18%)
2	3FG	I	7	2,6	9,13,13	2.76	3 (33%)	14,18,18	1.72	3 (21%)
2	GHP	J	1	2	10,11,12	2.58	1 (10%)	12,14,16	1.34	2 (16%)
2	3MY	J	2	2	11,13,14	2.88	3 (27%)	15,17,19	1.64	4 (26%)
2	3FG	J	3	2	11,12,13	2.33	5 (45%)	14,16,18	2.26	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GHP	J	4	2	10,11,12	2.88	5 (50%)	12,14,16	1.23	1 (8%)
2	GHP	J	5	2	10,11,12	2.33	1 (10%)	12,14,16	2.44	4 (33%)
2	OMY	J	6	2,7	13,14,15	2.77	8 (61%)	16,19,21	1.79	3 (18%)
2	3FG	J	7	2,6	9,13,13	3.25	6 (66%)	14,18,18	1.40	2 (14%)
2	GHP	K	1	2	10,11,12	2.93	2 (20%)	12,14,16	0.91	1 (8%)
2	3MY	K	2	2	11,13,14	3.26	3 (27%)	15,17,19	2.19	4 (26%)
2	3FG	K	3	2	11,12,13	2.72	2 (18%)	14,16,18	1.97	4 (28%)
2	GHP	K	4	8,2	10,11,12	1.90	2 (20%)	12,14,16	1.44	1 (8%)
2	GHP	K	5	2	10,11,12	3.34	2 (20%)	12,14,16	2.04	4 (33%)
2	OMY	K	6	2,7	13,14,15	2.34	6 (46%)	16,19,21	1.56	3 (18%)
2	3FG	K	7	2,6	9,13,13	2.47	3 (33%)	14,18,18	1.72	4 (28%)
2	GHP	L	1	2	10,11,12	2.76	2 (20%)	12,14,16	0.66	0
2	3MY	L	2	2	11,13,14	2.51	3 (27%)	15,17,19	2.19	4 (26%)
2	3FG	L	3	2	11,12,13	2.98	4 (36%)	14,16,18	1.88	4 (28%)
2	GHP	L	4	8,2	10,11,12	2.76	4 (40%)	12,14,16	1.37	2 (16%)
2	GHP	L	5	2	10,11,12	2.75	2 (20%)	12,14,16	3.03	6 (50%)
2	OMY	L	6	2,7	13,14,15	2.41	3 (23%)	16,19,21	1.96	5 (31%)
2	3FG	L	7	2,6	9,13,13	2.97	2 (22%)	14,18,18	1.97	5 (35%)
2	GHP	M	1	2	10,11,12	2.96	2 (20%)	12,14,16	1.28	2 (16%)
2	3MY	M	2	2	11,13,14	2.75	2 (18%)	15,17,19	2.81	5 (33%)
2	3FG	M	3	2	11,12,13	2.82	3 (27%)	14,16,18	1.65	2 (14%)
2	GHP	M	4	8,2	10,11,12	2.58	3 (30%)	12,14,16	1.23	1 (8%)
2	GHP	M	5	2	10,11,12	3.12	2 (20%)	12,14,16	2.22	6 (50%)
2	OMY	M	6	2,7	13,14,15	2.39	4 (30%)	16,19,21	1.74	4 (25%)
2	3FG	M	7	2,6	9,13,13	2.44	3 (33%)	14,18,18	2.44	2 (14%)
2	GHP	N	1	2	10,11,12	2.18	3 (30%)	12,14,16	1.19	0
2	3MY	N	2	2	11,13,14	2.68	2 (18%)	15,17,19	2.30	4 (26%)
2	3FG	N	3	2	11,12,13	2.14	3 (27%)	14,16,18	2.16	4 (28%)
2	GHP	N	4	8,2	10,11,12	3.22	2 (20%)	12,14,16	0.86	0
2	GHP	N	5	2	10,11,12	2.74	2 (20%)	12,14,16	2.12	4 (33%)
2	OMY	N	6	2,7	13,14,15	2.17	7 (53%)	16,19,21	1.46	3 (18%)
2	3FG	N	7	2,6	9,13,13	2.50	4 (44%)	14,18,18	1.35	2 (14%)
2	GHP	O	1	2	10,11,12	2.85	2 (20%)	12,14,16	0.80	0
2	3MY	O	2	2	11,13,14	1.96	2 (18%)	15,17,19	1.62	3 (20%)
2	3FG	O	3	2	11,12,13	1.55	2 (18%)	14,16,18	1.74	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GHP	O	4	8,2	10,11,12	2.70	2 (20%)	12,14,16	1.08	1 (8%)
2	GHP	O	5	2	10,11,12	2.88	5 (50%)	12,14,16	1.67	2 (16%)
2	OMY	O	6	2,7	13,14,15	2.24	5 (38%)	16,19,21	1.11	1 (6%)
2	3FG	O	7	2,6	9,13,13	2.73	3 (33%)	14,18,18	1.71	2 (14%)
2	GHP	P	1	2	10,11,12	3.25	6 (60%)	12,14,16	1.04	1 (8%)
2	3MY	P	2	2	11,13,14	2.01	6 (54%)	15,17,19	1.30	1 (6%)
2	3FG	P	3	2	11,12,13	2.01	4 (36%)	14,16,18	1.66	3 (21%)
2	GHP	P	4	8,2	10,11,12	1.73	3 (30%)	12,14,16	1.73	4 (33%)
2	GHP	P	5	2	10,11,12	3.04	1 (10%)	12,14,16	2.57	6 (50%)
2	OMY	P	6	2,7	13,14,15	1.92	2 (15%)	16,19,21	1.59	3 (18%)
2	3FG	P	7	2,6	9,13,13	2.95	3 (33%)	14,18,18	1.63	4 (28%)

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	GHP	I	1	2	-	0/4/6/8	0/1/1/1
2	3MY	I	2	2	-	0/4/6/8	0/1/1/1
2	3FG	I	3	2	-	0/4/6/8	0/1/1/1
2	GHP	I	4	2	-	0/4/6/8	0/1/1/1
2	GHP	I	5	2	-	0/4/6/8	0/1/1/1
2	OMY	I	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	I	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	J	1	2	-	0/4/6/8	0/1/1/1
2	3MY	J	2	2	-	0/4/6/8	0/1/1/1
2	3FG	J	3	2	-	0/4/6/8	0/1/1/1
2	GHP	J	4	2	-	0/4/6/8	0/1/1/1
2	GHP	J	5	2	-	0/4/6/8	0/1/1/1
2	OMY	J	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	J	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	K	1	2	-	0/4/6/8	0/1/1/1
2	3MY	K	2	2	-	0/4/6/8	0/1/1/1
2	3FG	K	3	2	-	0/4/6/8	0/1/1/1
2	GHP	K	4	8,2	-	0/4/6/8	0/1/1/1
2	GHP	K	5	2	-	0/4/6/8	0/1/1/1
2	OMY	K	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	K	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	L	1	2	-	0/4/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3MY	L	2	2	-	0/4/6/8	0/1/1/1
2	3FG	L	3	2	-	0/4/6/8	0/1/1/1
2	GHP	L	4	8,2	-	0/4/6/8	0/1/1/1
2	GHP	L	5	2	-	0/4/6/8	0/1/1/1
2	OMY	L	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	L	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	M	1	2	-	0/4/6/8	0/1/1/1
2	3MY	M	2	2	-	0/4/6/8	0/1/1/1
2	3FG	M	3	2	-	0/4/6/8	0/1/1/1
2	GHP	M	4	8,2	-	0/4/6/8	0/1/1/1
2	GHP	M	5	2	-	0/4/6/8	0/1/1/1
2	OMY	M	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	M	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	N	1	2	-	0/4/6/8	0/1/1/1
2	3MY	N	2	2	-	0/4/6/8	0/1/1/1
2	3FG	N	3	2	-	0/4/6/8	0/1/1/1
2	GHP	N	4	8,2	-	0/4/6/8	0/1/1/1
2	GHP	N	5	2	-	0/4/6/8	0/1/1/1
2	OMY	N	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	N	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	O	1	2	-	0/4/6/8	0/1/1/1
2	3MY	O	2	2	-	0/4/6/8	0/1/1/1
2	3FG	O	3	2	-	0/4/6/8	0/1/1/1
2	GHP	O	4	8,2	-	0/4/6/8	0/1/1/1
2	GHP	O	5	2	-	0/4/6/8	0/1/1/1
2	OMY	O	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	O	7	2,6	-	0/4/8/8	0/1/1/1
2	GHP	P	1	2	-	0/4/6/8	0/1/1/1
2	3MY	P	2	2	-	0/4/6/8	0/1/1/1
2	3FG	P	3	2	-	0/4/6/8	0/1/1/1
2	GHP	P	4	8,2	-	0/4/6/8	0/1/1/1
2	GHP	P	5	2	-	0/4/6/8	0/1/1/1
2	OMY	P	6	2,7	-	0/8/10/12	0/1/1/1
2	3FG	P	7	2,6	-	0/4/8/8	0/1/1/1

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	5	GHP	C1-CA	-9.76	1.41	1.52
2	M	5	GHP	C1-CA	-9.00	1.42	1.52
2	N	4	GHP	C1-CA	-8.89	1.42	1.52
2	K	1	GHP	C1-CA	-8.69	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	3FG	CB-CA	-8.63	1.42	1.52
2	P	5	GHP	C1-CA	-8.56	1.42	1.52
2	P	1	GHP	C1-CA	-8.50	1.42	1.52
2	M	1	GHP	C1-CA	-8.43	1.42	1.52
2	L	3	3FG	CB-CA	-8.36	1.42	1.52
2	I	1	GHP	C1-CA	-8.26	1.42	1.52
2	I	5	GHP	C1-CA	-8.12	1.43	1.52
2	O	1	GHP	C1-CA	-7.95	1.43	1.52
2	K	3	3FG	CB-CA	-7.89	1.43	1.52
2	N	5	GHP	C1-CA	-7.80	1.43	1.52
2	M	3	3FG	CB-CA	-7.78	1.43	1.52
2	P	7	3FG	CB-CA	-7.64	1.43	1.52
2	L	7	3FG	CB-CA	-7.59	1.43	1.52
2	O	4	GHP	C1-CA	-7.59	1.43	1.52
2	L	5	GHP	C1-CA	-7.55	1.43	1.52
2	L	1	GHP	C1-CA	-7.53	1.43	1.52
2	J	4	GHP	C1-CA	-7.28	1.44	1.52
2	L	4	GHP	C1-CA	-7.01	1.44	1.52
2	J	1	GHP	C1-CA	-6.89	1.44	1.52
2	M	4	GHP	C1-CA	-6.89	1.44	1.52
2	O	5	GHP	C1-CA	-6.64	1.44	1.52
2	L	6	OMY	CG-CB	-6.38	1.42	1.51
2	J	5	GHP	C1-CA	-6.29	1.45	1.52
2	M	6	OMY	CG-CB	-6.21	1.42	1.51
2	K	7	3FG	CB-CA	-6.19	1.45	1.52
2	O	7	3FG	CB-CA	-6.19	1.45	1.52
2	K	2	3MY	CB-CG	-5.62	1.37	1.51
2	I	6	OMY	CG-CB	-5.55	1.43	1.51
2	I	7	3FG	CB-CA	-5.54	1.46	1.52
2	N	3	3FG	CB-CA	-5.46	1.46	1.52
2	I	4	GHP	C1-CA	-5.43	1.46	1.52
2	M	7	3FG	CB-CA	-5.26	1.46	1.52
2	P	6	OMY	CG-CB	-5.23	1.43	1.51
2	K	6	OMY	CG-CB	-5.04	1.44	1.51
2	M	2	3MY	CB-CG	-4.96	1.39	1.51
2	N	7	3FG	CB-CA	-4.87	1.46	1.52
2	N	1	GHP	C1-CA	-4.72	1.47	1.52
2	K	4	GHP	C1-CA	-4.65	1.47	1.52
2	O	6	OMY	CG-CB	-4.61	1.44	1.51
2	P	3	3FG	CB-CA	-4.59	1.47	1.52
2	N	6	OMY	CG-CB	-4.53	1.44	1.51
2	J	7	3FG	CB-CA	-4.33	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	3MY	CB-CG	-4.32	1.40	1.51
2	I	2	3MY	CB-CG	-4.32	1.40	1.51
2	L	2	3MY	CB-CG	-4.07	1.41	1.51
2	J	2	3MY	CB-CG	-4.04	1.41	1.51
2	N	2	3MY	CB-CG	-3.67	1.42	1.51
2	N	4	GHP	CA-C	-3.59	1.39	1.50
2	J	3	3FG	CB-CA	-3.54	1.48	1.52
2	J	6	OMY	CG-CB	-3.53	1.46	1.51
2	I	3	3FG	CA-C	-3.39	1.40	1.50
2	L	3	3FG	CA-C	-3.39	1.40	1.50
2	M	3	3FG	CA-C	-3.33	1.40	1.50
2	L	5	GHP	CA-C	-3.32	1.40	1.50
2	K	5	GHP	CA-C	-3.13	1.41	1.50
2	P	4	GHP	C1-CA	-3.11	1.48	1.52
2	P	2	3MY	CB-CG	-3.06	1.43	1.51
2	L	4	GHP	CA-C	-2.86	1.41	1.50
2	M	5	GHP	CA-C	-2.84	1.42	1.50
2	P	4	GHP	CA-C	-2.78	1.42	1.50
2	I	4	GHP	CA-C	-2.52	1.42	1.50
2	K	1	GHP	CA-C	-2.40	1.43	1.50
2	N	6	OMY	CE1-CL	-2.31	1.67	1.73
2	J	7	3FG	OD2-CD2	-2.27	1.31	1.37
2	P	3	3FG	CA-C	-2.24	1.43	1.50
2	M	4	GHP	CA-C	-2.23	1.43	1.50
2	N	3	3FG	CA-C	-2.22	1.43	1.50
2	J	4	GHP	CA-C	-2.18	1.43	1.50
2	K	3	3FG	CA-C	-2.09	1.44	1.50
2	K	6	OMY	OCZ-CZ	2.00	1.40	1.36
2	L	2	3MY	CD2-CE2	2.01	1.42	1.38
2	P	1	GHP	C6-C1	2.01	1.42	1.39
2	K	7	3FG	CG2-CB	2.02	1.42	1.39
2	P	1	GHP	C3-C4	2.02	1.42	1.38
2	L	3	3FG	OD2-CD2	2.03	1.41	1.37
2	M	1	GHP	C2-C1	2.04	1.42	1.39
2	P	4	GHP	C3-C2	2.05	1.42	1.38
2	O	6	OMY	CZ-CE1	2.05	1.41	1.39
2	O	6	OMY	CD2-CG	2.06	1.42	1.39
2	L	3	3FG	CZ-CD1	2.08	1.42	1.39
2	M	7	3FG	CG2-CB	2.11	1.42	1.39
2	N	6	OMY	CD2-CG	2.11	1.42	1.39
2	P	7	3FG	CG1-CD1	2.11	1.42	1.39
2	J	4	GHP	C2-C1	2.11	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	OMY	CA-CB	2.12	1.58	1.54
2	M	4	GHP	C6-C5	2.13	1.43	1.38
2	O	5	GHP	C3-C4	2.15	1.43	1.38
2	P	1	GHP	C2-C1	2.16	1.42	1.39
2	K	2	3MY	CD2-CE2	2.17	1.42	1.38
2	L	4	GHP	C2-C1	2.17	1.42	1.39
2	I	2	3MY	OBD-CZ	2.18	1.40	1.36
2	K	6	OMY	CD2-CG	2.18	1.42	1.39
2	N	6	OMY	ODE-CB	2.18	1.47	1.42
2	P	3	3FG	CG2-CB	2.20	1.42	1.39
2	N	5	GHP	C3-C2	2.20	1.43	1.38
2	O	1	GHP	C3-C2	2.20	1.43	1.38
2	J	4	GHP	C6-C5	2.22	1.43	1.38
2	O	5	GHP	C6-C5	2.22	1.43	1.38
2	M	3	3FG	CZ-CD1	2.23	1.42	1.39
2	O	5	GHP	C5-C4	2.24	1.43	1.38
2	J	6	OMY	OCZ-CZ	2.25	1.41	1.36
2	J	6	OMY	CD2-CG	2.25	1.42	1.39
2	L	1	GHP	C2-C1	2.25	1.42	1.39
2	K	4	GHP	C6-C5	2.25	1.43	1.38
2	N	6	OMY	CA-N	2.29	1.54	1.47
2	P	2	3MY	CZ-CE2	2.29	1.41	1.39
2	I	5	GHP	C3-C4	2.30	1.43	1.38
2	P	1	GHP	C6-C5	2.32	1.43	1.38
2	O	3	3FG	CG2-CD2	2.33	1.42	1.39
2	P	1	GHP	C3-C2	2.34	1.43	1.38
2	P	3	3FG	CG2-CD2	2.35	1.42	1.39
2	N	1	GHP	C2-C1	2.36	1.42	1.39
2	P	2	3MY	CE2-CL	2.36	1.79	1.73
2	O	4	GHP	C6-C1	2.36	1.42	1.39
2	P	2	3MY	CD1-CE1	2.41	1.43	1.38
2	N	3	3FG	OD2-CD2	2.42	1.42	1.37
2	L	4	GHP	C3-C2	2.42	1.43	1.38
2	N	7	3FG	CG2-CB	2.43	1.42	1.39
2	O	6	OMY	OCZ-CZ	2.43	1.41	1.36
2	N	6	OMY	CZ-CE1	2.47	1.41	1.39
2	I	4	GHP	C3-C4	2.47	1.43	1.38
2	I	6	OMY	CA-N	2.47	1.55	1.47
2	N	1	GHP	C6-C1	2.57	1.43	1.39
2	P	2	3MY	OBD-CZ	2.58	1.41	1.36
2	I	6	OMY	CD2-CG	2.62	1.43	1.39
2	K	6	OMY	CA-CB	2.63	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	7	3FG	CG2-CB	2.65	1.43	1.39
2	M	6	OMY	CZ-CE1	2.65	1.42	1.39
2	J	6	OMY	CA-N	2.66	1.55	1.47
2	P	2	3MY	CD1-CG	2.67	1.44	1.38
2	J	4	GHP	C3-C2	2.71	1.44	1.38
2	O	3	3FG	CG2-CB	2.80	1.43	1.39
2	J	3	3FG	CG1-CD1	2.87	1.43	1.39
2	J	3	3FG	CG2-CD2	2.89	1.43	1.39
2	O	2	3MY	CE2-CL	2.89	1.81	1.73
2	N	7	3FG	CG1-CB	2.90	1.43	1.39
2	I	6	OMY	CZ-CE1	2.94	1.42	1.39
2	K	7	3FG	CG1-CB	2.98	1.43	1.39
2	P	7	3FG	CG1-CB	2.99	1.43	1.39
2	J	7	3FG	CZ-CD1	2.99	1.43	1.39
2	M	6	OMY	CE1-CL	3.00	1.81	1.73
2	J	3	3FG	CG2-CB	3.02	1.43	1.39
2	N	7	3FG	CG1-CD1	3.11	1.44	1.39
2	J	3	3FG	OD2-CD2	3.25	1.44	1.37
2	P	6	OMY	O-C	3.30	1.35	1.19
2	J	7	3FG	CG1-CD1	3.40	1.44	1.39
2	N	6	OMY	O-C	3.48	1.35	1.19
2	L	6	OMY	CZ-CE1	3.55	1.42	1.39
2	J	6	OMY	CA-CB	3.57	1.60	1.54
2	J	6	OMY	CE1-CL	3.64	1.83	1.73
2	K	6	OMY	CZ-CE1	3.65	1.42	1.39
2	I	6	OMY	CE1-CL	3.68	1.83	1.73
2	L	7	3FG	CG1-CB	3.71	1.45	1.39
2	K	6	OMY	O-C	3.74	1.37	1.19
2	L	6	OMY	O-C	3.80	1.37	1.19
2	O	7	3FG	CG1-CB	3.81	1.45	1.39
2	O	5	GHP	C6-C1	3.82	1.45	1.39
2	J	6	OMY	O-C	3.84	1.37	1.19
2	M	6	OMY	O-C	3.85	1.37	1.19
2	M	7	3FG	CG1-CB	3.95	1.45	1.39
2	I	7	3FG	CG1-CD1	3.96	1.45	1.39
2	I	6	OMY	O-C	3.99	1.38	1.19
2	O	6	OMY	O-C	4.01	1.38	1.19
2	I	7	3FG	CG1-CB	4.01	1.45	1.39
2	J	6	OMY	CZ-CE1	4.59	1.43	1.39
2	J	7	3FG	CG2-CB	4.70	1.46	1.39
2	I	2	3MY	CZ-CE2	4.77	1.44	1.39
2	J	7	3FG	CG1-CB	5.03	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	3MY	CZ-CE2	5.46	1.44	1.39
2	J	2	3MY	CE2-CL	5.64	1.88	1.73
2	L	2	3MY	CE2-CL	6.35	1.90	1.73
2	N	2	3MY	CE2-CL	7.07	1.91	1.73
2	M	2	3MY	CE2-CL	7.14	1.92	1.73
2	K	2	3MY	CE2-CL	8.72	1.96	1.73

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	2	3MY	CD2-CE2-CZ	-8.05	116.58	121.15
2	K	2	3MY	CD2-CE2-CZ	-5.98	117.75	121.15
2	L	5	GHP	C-CA-N	-5.94	95.67	109.14
2	I	2	3MY	CD2-CE2-CL	-5.08	110.23	118.46
2	L	2	3MY	CD2-CE2-CZ	-4.88	118.37	121.15
2	P	5	GHP	C5-C6-C1	-4.82	116.22	121.20
2	K	5	GHP	C-CA-N	-4.63	98.64	109.14
2	N	2	3MY	CD2-CE2-CZ	-4.56	118.56	121.15
2	L	6	OMY	C-CA-N	-4.52	99.99	109.95
2	K	6	OMY	C-CA-N	-4.27	100.52	109.95
2	M	7	3FG	CB-CA-N	-4.12	101.78	112.92
2	M	6	OMY	CD1-CE1-CZ	-4.09	118.82	121.15
2	N	2	3MY	CG-CB-CA	-3.94	105.03	114.12
2	J	5	GHP	C2-C3-C4	-3.91	115.38	119.86
2	K	4	GHP	C-CA-N	-3.82	100.48	109.14
2	P	5	GHP	C2-C3-C4	-3.75	115.56	119.86
2	I	6	OMY	CD1-CE1-CZ	-3.61	119.10	121.15
2	J	3	3FG	CG2-CD2-CZ	-3.52	115.16	120.43
2	P	6	OMY	ODE-CB-CA	-3.50	98.64	107.44
2	N	5	GHP	C2-C3-C4	-3.46	115.89	119.86
2	J	7	3FG	CD1-CG1-CB	-3.41	117.06	120.15
2	K	7	3FG	CB-CA-N	-3.38	103.79	112.92
2	L	5	GHP	C2-C3-C4	-3.38	115.99	119.86
2	O	2	3MY	CE2-CD2-CG	-3.31	118.66	120.46
2	L	7	3FG	CB-CA-N	-3.31	103.99	112.92
2	K	3	3FG	CB-CA-N	-3.27	104.89	112.53
2	L	6	OMY	O-C-CA	-3.25	116.81	125.69
2	L	4	GHP	C-CA-N	-3.25	101.77	109.14
2	N	6	OMY	O-C-CA	-3.24	116.83	125.69
2	L	6	OMY	CD1-CE1-CZ	-3.22	119.32	121.15
2	J	6	OMY	O-C-CA	-3.03	117.42	125.69
2	O	3	3FG	CB-CA-N	-2.96	105.60	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	3	3FG	CB-CA-N	-2.93	105.68	112.53
2	I	6	OMY	O-C-CA	-2.91	117.74	125.69
2	L	7	3FG	CD1-CG1-CB	-2.90	117.52	120.15
2	P	7	3FG	CB-CA-N	-2.87	105.16	112.92
2	P	6	OMY	O-C-CA	-2.84	117.94	125.69
2	I	5	GHP	C2-C3-C4	-2.80	116.65	119.86
2	M	5	GHP	C2-C1-CA	-2.79	115.81	120.70
2	P	7	3FG	CD1-CG1-CB	-2.75	117.66	120.15
2	J	5	GHP	C5-C6-C1	-2.73	118.38	121.20
2	O	7	3FG	CD1-CG1-CB	-2.70	117.71	120.15
2	M	6	OMY	C-CA-N	-2.70	104.00	109.95
2	K	6	OMY	O-C-CA	-2.67	118.41	125.69
2	N	3	3FG	CB-CA-N	-2.66	106.31	112.53
2	M	1	GHP	C2-C3-C4	-2.64	116.83	119.86
2	K	5	GHP	C2-C1-CA	-2.63	116.09	120.70
2	M	5	GHP	C-CA-N	-2.62	103.20	109.14
2	K	2	3MY	O-C-CA	-2.58	118.81	125.72
2	J	2	3MY	CD2-CE2-CL	-2.58	114.29	118.46
2	J	2	3MY	CD1-CE1-CZ	-2.57	117.92	120.50
2	M	2	3MY	O-C-CA	-2.57	118.84	125.72
2	L	2	3MY	O-C-CA	-2.56	118.85	125.72
2	K	3	3FG	CG2-CD2-CZ	-2.55	116.61	120.43
2	P	2	3MY	CD1-CE1-CZ	-2.51	117.99	120.50
2	J	1	GHP	C2-C3-C4	-2.50	116.99	119.86
2	M	4	GHP	C-CA-N	-2.50	103.47	109.14
2	I	3	3FG	CG2-CD2-CZ	-2.49	116.71	120.43
2	N	3	3FG	CG2-CD2-CZ	-2.48	116.71	120.43
2	P	4	GHP	C6-C5-C4	-2.48	117.01	119.86
2	M	5	GHP	C2-C3-C4	-2.47	117.03	119.86
2	L	3	3FG	CG2-CD2-CZ	-2.46	116.74	120.43
2	I	3	3FG	CB-CA-N	-2.43	106.85	112.53
2	M	6	OMY	O-C-CA	-2.40	119.14	125.69
2	I	2	3MY	CB-CG-CD2	-2.38	115.80	120.32
2	L	7	3FG	OD1-CD1-CG1	-2.38	113.53	119.80
2	O	6	OMY	O-C-CA	-2.33	119.31	125.69
2	O	4	GHP	C2-C3-C4	-2.32	117.21	119.86
2	N	6	OMY	CD2-CE2-CZ	-2.31	118.19	120.50
2	P	5	GHP	O4-C4-C3	-2.30	113.55	120.04
2	K	1	GHP	C2-C3-C4	-2.27	117.26	119.86
2	K	7	3FG	OD1-CD1-CG1	-2.25	113.89	119.80
2	N	7	3FG	CD1-CG1-CB	-2.24	118.12	120.15
2	I	5	GHP	C2-C1-CA	-2.23	116.78	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	5	GHP	O4-C4-C3	-2.17	113.92	120.04
2	P	7	3FG	OD1-CD1-CG1	-2.17	114.10	119.80
2	L	6	OMY	CD2-CE2-CZ	-2.17	118.33	120.50
2	P	3	3FG	CB-CA-N	-2.16	107.48	112.53
2	P	4	GHP	C6-C1-C2	-2.14	115.59	118.30
2	I	7	3FG	CB-CA-N	-2.08	107.29	112.92
2	L	5	GHP	C2-C1-CA	-2.06	117.08	120.70
2	O	5	GHP	C2-C1-CA	-2.01	117.17	120.70
2	K	6	OMY	CD2-CG-CB	2.03	123.81	120.72
2	M	1	GHP	C-CA-N	2.07	113.83	109.14
2	N	6	OMY	ODE-CB-CG	2.09	115.86	111.22
2	P	5	GHP	C5-C4-C3	2.11	122.69	119.78
2	P	6	OMY	CD1-CE1-CZ	2.12	122.35	121.15
2	K	7	3FG	CG2-CB-CA	2.13	122.06	119.54
2	J	2	3MY	CE1-CZ-CE2	2.15	120.71	118.45
2	J	2	3MY	CZ-CE2-CL	2.20	125.51	119.53
2	P	1	GHP	C1-CA-N	2.23	117.75	112.53
2	J	4	GHP	C1-CA-N	2.27	117.84	112.53
2	O	2	3MY	OBD-CZ-CE1	2.27	125.54	119.36
2	O	3	3FG	CD2-CG2-CB	2.29	122.22	120.15
2	J	3	3FG	CG1-CB-CA	2.32	122.88	119.74
2	K	5	GHP	C6-C1-CA	2.33	124.79	120.70
2	N	5	GHP	C5-C4-C3	2.34	122.99	119.78
2	L	5	GHP	C6-C1-CA	2.37	124.86	120.70
2	J	1	GHP	C3-C2-C1	2.40	123.68	121.20
2	M	2	3MY	CE2-CD2-CG	2.41	121.76	120.46
2	N	7	3FG	CD2-CG2-CB	2.43	122.35	120.15
2	P	7	3FG	C-CA-CB	2.44	114.55	111.25
2	M	6	OMY	CE2-CZ-CE1	2.45	121.02	118.45
2	N	2	3MY	CD1-CG-CD2	2.46	122.08	118.53
2	L	4	GHP	C2-C1-CA	2.46	125.02	120.70
2	J	7	3FG	C-CA-CB	2.47	114.58	111.25
2	L	7	3FG	CG1-CB-CA	2.49	122.48	119.54
2	I	3	3FG	CG2-CB-CA	2.50	123.12	119.74
2	O	3	3FG	CG1-CB-CA	2.51	123.13	119.74
2	O	2	3MY	CD2-CE2-CL	2.53	122.55	118.46
2	M	5	GHP	C3-C2-C1	2.54	123.83	121.20
2	L	6	OMY	CE2-CZ-CE1	2.57	121.14	118.45
2	I	6	OMY	CD2-CG-CB	2.57	124.63	120.72
2	K	2	3MY	CE1-CZ-CE2	2.58	121.16	118.45
2	P	5	GHP	C6-C1-C2	2.74	121.77	118.30
2	P	4	GHP	C2-C1-CA	2.74	125.50	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	5	GHP	C3-C2-C1	2.74	124.04	121.20
2	M	5	GHP	C6-C1-CA	2.77	125.56	120.70
2	K	5	GHP	C1-CA-N	3.01	119.56	112.53
2	N	3	3FG	C-CA-N	3.06	116.08	109.14
2	L	3	3FG	CD2-CG2-CB	3.08	122.93	120.15
2	J	6	OMY	CD2-CG-CB	3.08	125.40	120.72
2	I	7	3FG	C-CA-CB	3.19	115.55	111.25
2	I	7	3FG	CG1-CB-CA	3.27	123.42	119.54
2	P	3	3FG	CD2-CG2-CB	3.30	123.13	120.15
2	M	3	3FG	CD2-CG2-CB	3.30	123.13	120.15
2	L	2	3MY	CE1-CZ-CE2	3.34	121.95	118.45
2	J	5	GHP	C3-C2-C1	3.34	124.65	121.20
2	P	4	GHP	C5-C6-C1	3.39	124.70	121.20
2	M	3	3FG	C-CA-N	3.44	116.94	109.14
2	P	3	3FG	CG1-CB-CA	3.50	124.48	119.74
2	I	2	3MY	CZ-CE2-CL	3.60	129.32	119.53
2	L	7	3FG	C-CA-CB	3.61	116.12	111.25
2	M	2	3MY	CE1-CZ-CE2	3.67	122.30	118.45
2	K	7	3FG	C-CA-CB	3.67	116.20	111.25
2	O	3	3FG	CD1-CG1-CB	3.70	123.50	120.15
2	K	3	3FG	C-CA-N	3.71	117.56	109.14
2	O	5	GHP	C1-CA-N	3.79	121.40	112.53
2	I	3	3FG	CD2-CG2-CB	3.80	123.59	120.15
2	N	2	3MY	CE1-CZ-CE2	3.81	122.45	118.45
2	J	6	OMY	ODE-CB-CG	3.91	119.89	111.22
2	K	2	3MY	CD2-CE2-CL	3.96	124.86	118.46
2	L	3	3FG	C-CA-N	3.99	118.18	109.14
2	O	7	3FG	C-CA-CB	4.01	116.66	111.25
2	P	5	GHP	C1-CA-N	4.07	122.06	112.53
2	M	2	3MY	CD2-CE2-CL	4.16	125.19	118.46
2	K	3	3FG	CD2-CG2-CB	4.20	123.95	120.15
2	L	2	3MY	CD2-CE2-CL	4.42	125.61	118.46
2	N	5	GHP	C1-CA-N	4.57	123.22	112.53
2	M	5	GHP	C1-CA-N	4.83	123.84	112.53
2	J	5	GHP	C1-CA-N	5.15	124.59	112.53
2	I	5	GHP	C1-CA-N	5.30	124.93	112.53
2	N	3	3FG	CD2-CG2-CB	5.35	124.99	120.15
2	I	3	3FG	C-CA-N	5.76	122.20	109.14
2	J	3	3FG	CD2-CG2-CB	6.22	125.77	120.15
2	L	5	GHP	C1-CA-N	6.45	127.63	112.53
2	M	7	3FG	C-CA-CB	7.23	121.00	111.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	GHP	1	0
2	I	3	3FG	2	0
2	K	2	3MY	1	0
2	L	1	GHP	1	0
2	L	2	3MY	1	0
2	L	3	3FG	1	0
2	L	6	OMY	1	0
2	M	6	OMY	1	0
2	N	2	3MY	5	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

37 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	A	601	1	52,58,58	1.68	12 (23%)	52,89,89	2.39	14 (26%)
4	CIT	A	602	-	3,12,12	1.49	1 (33%)	3,17,17	1.54	1 (33%)
3	FAD	B	601	1	52,58,58	1.42	6 (11%)	52,89,89	2.98	15 (28%)
5	T55	B	602	8	10,10,11	0.55	0	10,10,12	1.24	1 (10%)
4	CIT	B	603	-	3,12,12	1.46	0	3,17,17	2.48	2 (66%)
3	FAD	C	601	1	52,58,58	1.64	8 (15%)	52,89,89	2.77	14 (26%)
4	CIT	C	602	-	3,12,12	1.07	0	3,17,17	1.98	2 (66%)
3	FAD	D	601	1	52,58,58	1.61	8 (15%)	52,89,89	2.66	16 (30%)
4	CIT	D	602	-	3,12,12	1.00	0	3,17,17	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	I	101	2	11,11,12	2.96	4 (36%)	15,15,17	2.88	4 (26%)
7	NAG	I	102	2	14,14,15	1.86	4 (28%)	15,19,21	2.03	7 (46%)
6	MAN	J	101	2	11,11,12	3.27	6 (54%)	15,15,17	1.71	1 (6%)
7	NAG	J	102	2	14,14,15	2.70	6 (42%)	15,19,21	3.23	9 (60%)
5	T55	K	101	8	10,10,11	0.61	0	10,10,12	0.94	0
6	MAN	K	102	2	11,11,12	1.21	1 (9%)	15,15,17	2.23	4 (26%)
7	NAG	K	103	2	14,14,15	0.99	1 (7%)	15,19,21	1.45	5 (33%)
8	N1L	K	104	2,5	9,12,13	3.91	5 (55%)	10,17,19	1.45	2 (20%)
6	MAN	L	101	2	11,11,12	0.74	0	15,15,17	1.12	1 (6%)
7	NAG	L	102	2	14,14,15	0.88	1 (7%)	15,19,21	1.60	3 (20%)
8	N1L	L	103	2,5	9,12,13	3.25	4 (44%)	10,17,19	1.48	2 (20%)
5	T55	M	101	8	10,10,11	0.65	0	10,10,12	1.23	2 (20%)
6	MAN	M	102	2	11,11,12	1.75	2 (18%)	15,15,17	1.83	2 (13%)
7	NAG	M	103	2	14,14,15	1.06	1 (7%)	15,19,21	1.30	2 (13%)
8	N1L	M	104	2,5	9,12,13	4.36	7 (77%)	10,17,19	2.72	5 (50%)
5	T55	N	101	8	10,10,11	0.66	0	10,10,12	1.53	3 (30%)
6	MAN	N	102	2	11,11,12	2.27	4 (36%)	15,15,17	1.55	4 (26%)
7	NAG	N	103	2	14,14,15	1.26	1 (7%)	15,19,21	1.52	3 (20%)
8	N1L	N	104	2,5	9,12,13	4.03	4 (44%)	10,17,19	1.65	2 (20%)
5	T55	O	101	8	10,10,11	0.75	0	10,10,12	0.64	0
6	MAN	O	102	2	11,11,12	2.43	4 (36%)	15,15,17	1.49	4 (26%)
7	NAG	O	103	2	14,14,15	1.38	2 (14%)	15,19,21	1.66	3 (20%)
8	N1L	O	104	2,5	9,12,13	3.81	4 (44%)	10,17,19	1.70	2 (20%)
4	CIT	O	105	-	3,12,12	1.92	1 (33%)	3,17,17	4.19	2 (66%)
5	T55	P	101	8	10,10,11	1.16	1 (10%)	10,10,12	0.62	0
6	MAN	P	102	2	11,11,12	1.68	3 (27%)	15,15,17	1.62	4 (26%)
7	NAG	P	103	2	14,14,15	2.10	4 (28%)	15,19,21	1.36	2 (13%)
8	N1L	P	104	2,5	9,12,13	3.89	6 (66%)	10,17,19	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	601	1	-	0/30/50/50	0/6/6/6
4	CIT	A	602	-	-	0/6/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	601	1	-	0/30/50/50	0/6/6/6
5	T55	B	602	8	-	0/7/8/9	0/0/0/0
4	CIT	B	603	-	-	0/6/16/16	0/0/0/0
3	FAD	C	601	1	-	0/30/50/50	0/6/6/6
4	CIT	C	602	-	-	0/6/16/16	0/0/0/0
3	FAD	D	601	1	-	0/30/50/50	0/6/6/6
4	CIT	D	602	-	-	0/6/16/16	0/0/0/0
6	MAN	I	101	2	-	0/2/19/22	0/1/1/1
7	NAG	I	102	2	-	0/6/23/26	0/1/1/1
6	MAN	J	101	2	-	0/2/19/22	0/1/1/1
7	NAG	J	102	2	-	0/6/23/26	0/1/1/1
5	T55	K	101	8	-	0/7/8/9	0/0/0/0
6	MAN	K	102	2	-	0/2/19/22	0/1/1/1
7	NAG	K	103	2	-	0/6/23/26	0/1/1/1
8	N1L	K	104	2,5	-	0/0/21/24	0/1/1/1
6	MAN	L	101	2	-	0/2/19/22	0/1/1/1
7	NAG	L	102	2	-	0/6/23/26	0/1/1/1
8	N1L	L	103	2,5	-	0/0/21/24	0/1/1/1
5	T55	M	101	8	-	0/7/8/9	0/0/0/0
6	MAN	M	102	2	-	0/2/19/22	1/1/1/1
7	NAG	M	103	2	-	0/6/23/26	0/1/1/1
8	N1L	M	104	2,5	-	0/0/21/24	0/1/1/1
5	T55	N	101	8	-	0/7/8/9	0/0/0/0
6	MAN	N	102	2	-	0/2/19/22	0/1/1/1
7	NAG	N	103	2	-	0/6/23/26	0/1/1/1
8	N1L	N	104	2,5	-	0/0/21/24	0/1/1/1
5	T55	O	101	8	-	0/7/8/9	0/0/0/0
6	MAN	O	102	2	-	0/2/19/22	0/1/1/1
7	NAG	O	103	2	-	0/6/23/26	0/1/1/1
8	N1L	O	104	2,5	-	0/0/21/24	0/1/1/1
4	CIT	O	105	-	-	0/6/16/16	0/0/0/0
5	T55	P	101	8	-	0/7/8/9	0/0/0/0
6	MAN	P	102	2	-	0/2/19/22	0/1/1/1
7	NAG	P	103	2	-	0/6/23/26	0/1/1/1
8	N1L	P	104	2,5	-	0/0/21/24	0/1/1/1

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	104	N1L	C2-N2	-4.20	1.32	1.47
8	N	104	N1L	C2-N2	-3.85	1.33	1.47
8	O	104	N1L	C2-N2	-3.80	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	104	N1L	C2-N2	-3.78	1.33	1.47
6	O	102	MAN	O4-C4	-2.70	1.36	1.43
8	M	104	N1L	C4-C3	-2.65	1.45	1.52
3	A	601	FAD	C2B-C1B	-2.49	1.49	1.53
3	A	601	FAD	C2'-C3'	-2.40	1.48	1.53
6	O	102	MAN	O2-C2	-2.37	1.38	1.43
3	D	601	FAD	C2B-C1B	-2.30	1.50	1.53
3	A	601	FAD	PA-O2A	-2.08	1.46	1.55
8	P	104	N1L	O4-C4	2.02	1.47	1.43
3	D	601	FAD	C6-C7	2.02	1.43	1.37
6	N	102	MAN	C2-C3	2.03	1.55	1.52
4	A	602	CIT	O7-C3	2.06	1.46	1.43
7	M	103	NAG	C8-C7	2.09	1.54	1.50
3	B	601	FAD	C8M-C8	2.16	1.55	1.51
8	P	104	N1L	C3-C2	2.20	1.58	1.53
7	P	103	NAG	C4-C5	2.20	1.57	1.53
6	J	101	MAN	O2-C2	2.21	1.48	1.43
8	M	104	N1L	C3-C2	2.24	1.58	1.53
3	A	601	FAD	C7M-C7	2.25	1.55	1.51
6	N	102	MAN	C4-C3	2.33	1.58	1.52
3	C	601	FAD	C6-C7	2.34	1.44	1.37
7	I	102	NAG	O5-C5	2.34	1.48	1.43
7	O	103	NAG	O5-C1	2.37	1.47	1.43
8	L	103	N1L	O3-C3	2.41	1.48	1.43
8	M	104	N1L	O5-C5	2.42	1.46	1.43
7	J	102	NAG	C2-N2	2.42	1.50	1.46
7	K	103	NAG	C8-C7	2.42	1.55	1.50
3	C	601	FAD	O4B-C1B	2.49	1.44	1.41
3	A	601	FAD	C2A-N3A	2.51	1.36	1.32
4	O	105	CIT	C4-C3	2.54	1.58	1.54
3	C	601	FAD	C8M-C8	2.55	1.56	1.51
6	P	102	MAN	O3-C3	2.57	1.49	1.43
7	I	102	NAG	C3-C2	2.57	1.58	1.52
7	P	103	NAG	C2-N2	2.58	1.50	1.46
6	P	102	MAN	C4-C3	2.62	1.59	1.52
3	A	601	FAD	C9A-N10	2.64	1.42	1.38
7	J	102	NAG	C3-C2	2.66	1.58	1.52
3	B	601	FAD	C6-C7	2.69	1.45	1.37
6	J	101	MAN	C4-C5	2.69	1.59	1.53
7	J	102	NAG	C8-C7	2.69	1.56	1.50
5	P	101	T55	CAL-C	2.72	1.57	1.49
7	L	102	NAG	C2-N2	2.74	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	103	NAG	C2-N2	2.78	1.51	1.46
3	A	601	FAD	C5A-C4A	2.79	1.46	1.40
7	O	103	NAG	C8-C7	2.83	1.56	1.50
3	C	601	FAD	C9A-N10	2.92	1.43	1.38
3	C	601	FAD	C4X-N5	2.94	1.37	1.33
6	K	102	MAN	O5-C1	2.94	1.48	1.43
6	J	101	MAN	C1-C2	2.99	1.59	1.52
7	P	103	NAG	O3-C3	2.99	1.50	1.43
3	A	601	FAD	C4-C4X	2.99	1.47	1.41
3	D	601	FAD	C4X-C10	3.03	1.46	1.40
3	A	601	FAD	C4X-C10	3.07	1.46	1.40
6	J	101	MAN	C4-C3	3.08	1.60	1.52
3	D	601	FAD	C8M-C8	3.09	1.57	1.51
3	B	601	FAD	C4X-C10	3.11	1.46	1.40
3	B	601	FAD	C4-C4X	3.11	1.47	1.41
8	O	104	N1L	C3-C2	3.12	1.60	1.53
7	I	102	NAG	C8-C7	3.15	1.57	1.50
6	N	102	MAN	O5-C5	3.17	1.50	1.43
3	B	601	FAD	C9A-C5X	3.20	1.49	1.42
6	O	102	MAN	O3-C3	3.30	1.50	1.43
3	A	601	FAD	C4X-N5	3.32	1.38	1.33
8	N	104	N1L	O5-C1	3.42	1.49	1.43
6	P	102	MAN	O5-C1	3.43	1.49	1.43
8	K	104	N1L	O3-C3	3.46	1.51	1.43
6	I	101	MAN	C1-C2	3.47	1.60	1.52
3	D	601	FAD	C4-C4X	3.50	1.48	1.41
7	I	102	NAG	O5-C1	3.54	1.49	1.43
8	P	104	N1L	O3-C3	3.72	1.51	1.43
6	M	102	MAN	O5-C1	3.72	1.49	1.43
8	K	104	N1L	O4-C4	3.89	1.52	1.43
6	M	102	MAN	O5-C5	3.94	1.52	1.43
6	I	101	MAN	C2-C3	3.95	1.57	1.52
3	C	601	FAD	C8-C7	3.95	1.51	1.41
3	B	601	FAD	C8-C7	3.97	1.51	1.41
7	J	102	NAG	O5-C5	4.03	1.52	1.43
3	A	601	FAD	C8-C7	4.15	1.52	1.41
3	D	601	FAD	C8-C7	4.31	1.52	1.41
6	J	101	MAN	O5-C5	4.33	1.53	1.43
8	L	103	N1L	O5-C5	4.35	1.48	1.43
3	A	601	FAD	C9A-C5X	4.35	1.51	1.42
3	D	601	FAD	C9A-C5X	4.36	1.51	1.42
6	I	101	MAN	O5-C5	4.36	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	103	N1L	C1-C2	4.40	1.58	1.52
7	J	102	NAG	C1-C2	4.51	1.58	1.52
3	C	601	FAD	C9A-C5X	4.51	1.52	1.42
3	D	601	FAD	O4B-C1B	4.52	1.47	1.41
3	C	601	FAD	C4X-C10	4.71	1.49	1.40
8	K	104	N1L	O5-C5	4.97	1.48	1.43
6	N	102	MAN	O5-C1	5.36	1.52	1.43
8	M	104	N1L	O5-C1	5.48	1.52	1.43
8	K	104	N1L	O5-C1	5.53	1.52	1.43
6	O	102	MAN	O5-C1	5.55	1.52	1.43
8	M	104	N1L	O3-C3	5.73	1.56	1.43
7	P	103	NAG	C1-C2	5.81	1.60	1.52
8	P	104	N1L	O5-C5	5.81	1.49	1.43
7	J	102	NAG	O5-C1	6.52	1.54	1.43
6	I	101	MAN	O5-C1	6.56	1.54	1.43
8	O	104	N1L	O5-C5	6.72	1.50	1.43
8	L	103	N1L	O5-C1	6.87	1.54	1.43
8	O	104	N1L	C1-C2	7.09	1.61	1.52
8	N	104	N1L	O5-C5	7.18	1.51	1.43
8	K	104	N1L	C1-C2	7.32	1.61	1.52
6	J	101	MAN	O5-C1	7.63	1.56	1.43
8	P	104	N1L	C1-C2	7.74	1.62	1.52
8	N	104	N1L	C1-C2	7.80	1.62	1.52
8	M	104	N1L	C1-C2	8.14	1.62	1.52

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	FAD	N3A-C2A-N1A	-9.23	121.62	128.87
3	D	601	FAD	C4-C4X-C10	-8.57	114.46	119.94
3	C	601	FAD	N3A-C2A-N1A	-7.85	122.71	128.87
4	O	105	CIT	C3-C2-C1	-6.90	104.17	114.95
3	B	601	FAD	C4X-C10-N10	-6.56	115.75	120.52
3	D	601	FAD	N3A-C2A-N1A	-6.34	123.89	128.87
3	B	601	FAD	C4-C4X-C10	-6.07	116.06	119.94
3	A	601	FAD	N3A-C2A-N1A	-5.77	124.34	128.87
3	C	601	FAD	C4X-C4-N3	-5.26	116.65	123.52
8	M	104	N1L	O4-C4-C3	-5.19	98.65	110.36
3	B	601	FAD	C4X-C4-N3	-4.96	117.04	123.52
3	C	601	FAD	C4X-C10-N10	-4.95	116.92	120.52
3	A	601	FAD	C4-C4X-C10	-4.93	116.79	119.94
3	D	601	FAD	N3-C2-N1	-4.65	119.85	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	104	N1L	C3-C2-N2	-4.58	102.72	110.66
3	A	601	FAD	C1B-N9A-C4A	-4.32	121.98	126.81
3	B	601	FAD	N3-C2-N1	-4.21	120.60	127.69
7	O	103	NAG	C4-C3-C2	-4.09	105.00	111.34
3	C	601	FAD	C4-C4X-C10	-4.01	117.38	119.94
8	O	104	N1L	O3-C3-C2	-3.84	102.78	109.95
3	A	601	FAD	C4X-C4-N3	-3.80	118.56	123.52
3	A	601	FAD	C7-C6-C5X	-3.73	114.81	120.90
7	I	102	NAG	C1-O5-C5	-3.70	106.70	112.14
7	J	102	NAG	O5-C5-C4	-3.64	104.11	110.13
3	C	601	FAD	N3-C2-N1	-3.63	121.58	127.69
3	D	601	FAD	C4X-C10-N10	-3.59	117.91	120.52
8	N	104	N1L	O5-C5-C4	-3.54	102.74	108.51
8	N	104	N1L	O3-C3-C2	-3.48	103.46	109.95
4	B	603	CIT	C3-C2-C1	-3.46	109.55	114.95
8	M	104	N1L	O3-C3-C4	-3.27	102.98	110.36
3	A	601	FAD	C4X-C10-N10	-3.26	118.15	120.52
7	N	103	NAG	O6-C6-C5	-3.25	100.46	111.30
8	K	104	N1L	C4-C3-C2	-3.16	107.27	111.54
3	A	601	FAD	N3-C2-N1	-3.10	122.47	127.69
7	J	102	NAG	C6-C5-C4	-3.10	105.22	112.99
7	J	102	NAG	C4-C3-C2	-3.07	106.58	111.34
7	P	103	NAG	O6-C6-C5	-3.07	101.06	111.30
8	L	103	N1L	O4-C4-C3	-3.07	103.44	110.36
3	D	601	FAD	C1B-N9A-C4A	-3.05	123.40	126.81
6	O	102	MAN	O4-C4-C3	-2.99	103.61	110.36
3	B	601	FAD	C7-C6-C5X	-2.99	116.02	120.90
7	O	103	NAG	O6-C6-C5	-2.95	101.44	111.30
3	C	601	FAD	C7-C6-C5X	-2.95	116.09	120.90
7	K	103	NAG	O6-C6-C5	-2.79	101.99	111.30
6	M	102	MAN	O6-C6-C5	-2.73	102.17	111.30
8	O	104	N1L	O4-C4-C3	-2.66	104.37	110.36
7	M	103	NAG	O6-C6-C5	-2.60	102.63	111.30
3	C	601	FAD	C9A-C5X-N5	-2.58	117.97	122.18
3	B	601	FAD	O2'-C2'-C1'	-2.57	103.59	109.93
7	O	103	NAG	C1-O5-C5	-2.53	108.42	112.14
3	D	601	FAD	C7-C6-C5X	-2.52	116.79	120.90
4	C	602	CIT	C3-C2-C1	-2.47	111.09	114.95
5	M	101	T55	CAK-CAL-C	-2.47	106.50	113.35
6	P	102	MAN	O6-C6-C5	-2.47	103.07	111.30
5	B	602	T55	CAK-CAL-C	-2.44	106.56	113.35
3	B	601	FAD	C9A-C5X-N5	-2.42	118.23	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	601	FAD	C1'-C2'-C3'	-2.42	102.89	109.82
7	J	102	NAG	C3-C4-C5	-2.38	105.99	110.23
3	D	601	FAD	C4X-C4-N3	-2.31	120.50	123.52
6	I	101	MAN	C3-C4-C5	-2.27	106.18	110.23
4	O	105	CIT	C4-C3-C2	-2.24	104.30	109.85
7	N	103	NAG	O7-C7-C8	-2.20	118.02	122.07
5	M	101	T55	CAI-CAJ-CAK	-2.19	103.19	114.54
7	L	102	NAG	C6-C5-C4	-2.18	107.51	112.99
7	I	102	NAG	O7-C7-C8	-2.18	118.05	122.07
4	A	602	CIT	C3-C2-C1	-2.17	111.56	114.95
3	A	601	FAD	C9A-C5X-N5	-2.16	118.66	122.18
5	N	101	T55	CAF-CAE-CAD	-2.12	100.18	110.52
7	J	102	NAG	O7-C7-C8	-2.11	118.18	122.07
8	L	103	N1L	C4-C3-C2	-2.10	108.70	111.54
7	I	102	NAG	O6-C6-C5	-2.10	104.29	111.30
7	P	103	NAG	O7-C7-C8	-2.10	118.21	122.07
7	K	103	NAG	C6-C5-C4	-2.00	107.96	112.99
7	K	103	NAG	C2-N2-C7	2.04	125.77	123.11
7	K	103	NAG	O5-C5-C6	2.05	111.74	107.34
6	O	102	MAN	C1-O5-C5	2.11	115.24	112.14
3	D	601	FAD	O5B-PA-O1A	2.12	117.90	109.21
7	K	103	NAG	C8-C7-N2	2.14	120.20	116.10
6	L	101	MAN	O5-C5-C6	2.14	111.93	107.34
3	D	601	FAD	C6-C5X-C9A	2.19	121.52	119.11
6	K	102	MAN	O5-C1-C2	2.19	114.40	110.89
3	D	601	FAD	O4'-C4'-C5'	2.20	114.89	110.09
3	D	601	FAD	N6A-C6A-N1A	2.22	122.23	118.52
7	J	102	NAG	O3-C3-C2	2.22	114.12	109.37
7	M	103	NAG	C2-N2-C7	2.22	125.99	123.11
7	I	102	NAG	C2-N2-C7	2.25	126.04	123.11
3	B	601	FAD	C6-C5X-C9A	2.26	121.61	119.11
6	O	102	MAN	O5-C1-C2	2.27	114.53	110.89
7	J	102	NAG	C8-C7-N2	2.27	120.45	116.10
3	C	601	FAD	C4-C4X-N5	2.28	121.47	118.70
5	N	101	T55	CAF-CAE-CAG	2.29	127.48	111.40
8	K	104	N1L	C1-C2-C3	2.31	112.91	109.21
4	C	602	CIT	C3-C4-C5	2.32	118.57	114.95
5	N	101	T55	CAJ-CAK-CAL	2.33	123.25	113.79
8	M	104	N1L	O4-C4-C5	2.34	114.86	110.40
6	N	102	MAN	O2-C2-C1	2.35	113.95	109.23
8	M	104	N1L	C3-C4-C5	2.37	113.30	108.60
6	N	102	MAN	O5-C1-C2	2.37	114.69	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	CIT	C3-C4-C5	2.48	118.83	114.95
7	L	102	NAG	O5-C5-C6	2.53	112.75	107.34
7	J	102	NAG	C2-N2-C7	2.56	126.43	123.11
6	P	102	MAN	O3-C3-C4	2.57	116.16	110.36
7	I	102	NAG	C8-C7-N2	2.58	121.05	116.10
7	N	103	NAG	C2-N2-C7	2.59	126.48	123.11
7	I	102	NAG	C4-C3-C2	2.60	115.38	111.34
6	K	102	MAN	C1-C2-C3	2.65	112.76	109.55
6	N	102	MAN	C1-O5-C5	2.65	116.04	112.14
3	C	601	FAD	O4B-C1B-N9A	2.71	113.22	108.11
6	K	102	MAN	O5-C5-C6	2.75	113.22	107.34
3	B	601	FAD	C2A-N1A-C6A	2.76	123.69	118.77
6	N	102	MAN	O5-C5-C6	2.76	113.26	107.34
3	B	601	FAD	N6A-C6A-N1A	2.77	123.16	118.52
3	C	601	FAD	C6-C5X-C9A	2.79	122.19	119.11
3	B	601	FAD	O2A-PA-O3P	2.79	117.23	105.27
3	A	601	FAD	O4B-C1B-N9A	2.80	113.40	108.11
6	P	102	MAN	O5-C1-C2	2.98	115.66	110.89
6	O	102	MAN	O5-C5-C6	3.09	113.95	107.34
3	A	601	FAD	C6-C5X-C9A	3.11	122.53	119.11
3	A	601	FAD	C4-C4X-N5	3.16	122.55	118.70
7	L	102	NAG	C2-N2-C7	3.36	127.48	123.11
3	C	601	FAD	C1'-N10-C9A	3.50	122.88	118.83
3	B	601	FAD	C4-C4X-N5	3.52	122.98	118.70
7	I	102	NAG	O5-C5-C6	3.62	115.08	107.34
3	A	601	FAD	N6A-C6A-N1A	3.75	124.80	118.52
6	P	102	MAN	C1-O5-C5	3.79	117.71	112.14
3	C	601	FAD	N6A-C6A-N1A	4.15	125.47	118.52
3	D	601	FAD	C4-C4X-N5	4.15	123.75	118.70
3	D	601	FAD	C4X-N5-C5X	4.26	121.75	116.72
6	I	101	MAN	O5-C5-C6	4.65	117.30	107.34
3	A	601	FAD	C4X-N5-C5X	5.02	122.64	116.72
3	D	601	FAD	C1'-N10-C9A	5.03	124.66	118.83
6	M	102	MAN	C1-O5-C5	5.20	119.79	112.14
3	C	601	FAD	C4X-N5-C5X	5.59	123.31	116.72
6	I	101	MAN	C1-C2-C3	5.75	116.52	109.55
6	J	101	MAN	O5-C5-C6	5.85	119.87	107.34
3	B	601	FAD	C4X-N5-C5X	6.09	123.89	116.72
6	K	102	MAN	C1-O5-C5	6.76	122.08	112.14
6	I	101	MAN	C1-O5-C5	7.45	123.09	112.14
3	A	601	FAD	C4-N3-C2	8.23	122.03	115.16
3	D	601	FAD	C4-N3-C2	8.87	122.56	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	102	NAG	O5-C5-C6	9.53	127.75	107.34
3	C	601	FAD	C4-N3-C2	10.42	123.86	115.16
3	B	601	FAD	C4-N3-C2	11.33	124.61	115.16

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	102	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	602	T55	1	0
5	K	101	T55	1	0
8	K	104	N1L	1	0
7	L	102	NAG	3	0
8	L	103	N1L	2	0
5	M	101	T55	4	0
8	M	104	N1L	1	0
5	N	101	T55	14	0
5	P	101	T55	0	1

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	498/523 (95%)	-0.24	10 (2%) 68 75	12, 21, 42, 137	0
1	B	498/523 (95%)	-0.16	10 (2%) 68 75	14, 24, 48, 120	0
1	C	498/523 (95%)	-0.12	19 (3%) 44 54	17, 28, 52, 110	0
1	D	498/523 (95%)	0.28	35 (7%) 19 27	20, 39, 61, 109	0
2	I	0/7	-	-	-	-
2	J	0/7	-	-	-	-
2	K	0/7	-	-	-	-
2	L	0/7	-	-	-	-
2	M	0/7	-	-	-	-
2	N	0/7	-	-	-	-
2	O	0/7	-	-	-	-
2	P	0/7	-	-	-	-
All	All	1992/2148 (92%)	-0.06	74 (3%) 45 55	12, 27, 55, 137	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	GLY	9.1
1	D	357	ARG	8.3
1	D	302	PRO	8.3
1	B	356	GLY	7.2
1	D	356	GLY	6.7
1	A	357	ARG	6.4
1	C	355	PRO	6.3
1	B	357	ARG	6.3
1	D	355	PRO	6.0
1	D	303	GLY	5.9
1	D	304	MET	5.3
1	C	357	ARG	5.2
1	D	358	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	354	THR	5.0
1	D	26	CYS	4.9
1	C	302	PRO	4.6
1	D	301	VAL	4.5
1	A	356	GLY	4.5
1	D	359	GLY	4.3
1	B	354	THR	4.1
1	C	359	GLY	4.1
1	A	302	PRO	4.1
1	C	354	THR	4.1
1	D	305	GLY	4.0
1	C	356	GLY	4.0
1	D	433	ALA	4.0
1	A	355	PRO	3.8
1	D	378	ARG	3.8
1	D	202	ARG	3.7
1	D	434	ASN	3.6
1	B	302	PRO	3.6
1	D	436	GLY	3.6
1	C	303	GLY	3.5
1	B	26	CYS	3.4
1	B	303	GLY	3.4
1	C	26	CYS	3.3
1	D	482	GLY	3.2
1	A	26	CYS	3.1
1	D	457	GLY	3.1
1	D	487	GLY	3.1
1	D	435	PRO	3.1
1	B	305	GLY	3.0
1	C	358	GLY	2.9
1	B	355	PRO	2.9
1	C	119	SER	2.9
1	D	285	ASP	2.9
1	D	481	PRO	2.8
1	D	392	GLY	2.8
1	D	205	PRO	2.7
1	C	523	PRO	2.7
1	D	265	ALA	2.6
1	C	304	MET	2.6
1	A	354	THR	2.6
1	C	305	GLY	2.6
1	B	320	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	203	ASP	2.6
1	B	304	MET	2.5
1	D	523	PRO	2.5
1	A	303	GLY	2.5
1	A	436	GLY	2.5
1	D	471	ILE	2.4
1	C	481	PRO	2.4
1	D	400	LEU	2.4
1	D	353	SER	2.4
1	A	304	MET	2.4
1	C	297	ILE	2.4
1	D	194	ARG	2.3
1	C	38	ASP	2.3
1	D	488	VAL	2.2
1	C	202	ARG	2.2
1	C	434	ASN	2.2
1	D	437	ASN	2.1
1	C	86	VAL	2.0
1	D	189	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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^2)	Q<0.9
2	OMY	O	6	14/15	0.91	0.23	-	34,40,48,56	0
2	3FG	N	7	13/13	0.93	0.27	-	34,41,47,51	0
2	GHP	P	4	11/12	0.97	0.10	-	27,30,31,34	0
2	GHP	N	1	11/12	0.95	0.21	-	25,30,33,34	0
2	GHP	L	4	11/12	0.75	0.12	-	54,66,75,78	0
2	GHP	M	4	11/12	0.74	0.21	-	59,80,94,105	0
2	3FG	O	7	13/13	0.82	0.26	-	40,45,52,54	0
2	GHP	I	5	11/12	0.70	0.32	-	58,76,103,104	0
2	GHP	O	1	11/12	0.94	0.15	-	28,31,36,37	0
2	3FG	O	3	12/13	0.94	0.16	-	27,31,32,36	0
2	GHP	M	5	11/12	0.34	0.62	-	112,143,167,185	0
2	3FG	I	7	13/13	0.51	0.43	-	69,100,119,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GHP	O	5	11/12	0.92	0.17	-	27,34,40,40	0
2	OMY	I	6	14/15	0.81	0.36	-	57,70,75,79	0
2	3MY	P	2	13/14	0.94	0.21	-	28,31,35,46	0
2	GHP	N	5	11/12	0.94	0.21	-	29,32,36,38	0
2	3FG	J	3	12/13	0.90	0.29	-	43,50,53,66	0
2	OMY	K	6	14/15	0.54	0.36	-	91,123,147,148	0
2	OMY	M	6	14/15	0.62	0.42	-	88,128,160,170	0
2	3MY	K	2	13/14	0.83	0.16	-	50,56,66,112	0
2	3MY	O	2	13/14	0.90	0.22	-	29,33,35,43	0
2	3MY	L	2	13/14	0.87	0.16	-	52,62,72,104	0
2	GHP	I	4	11/12	0.86	0.21	-	41,50,55,55	0
2	3MY	N	2	13/14	0.91	0.20	-	25,33,40,58	0
2	GHP	J	5	11/12	0.88	0.25	-	45,50,56,60	0
2	3MY	J	2	13/14	0.84	0.34	-	44,55,65,77	0
2	3FG	K	3	12/13	0.85	0.19	-	58,72,78,80	0
2	3FG	M	7	13/13	0.15	0.79	-	116,143,162,171	0
2	GHP	K	5	11/12	0.41	0.55	-	108,137,152,169	0
2	3FG	K	7	13/13	0.42	0.70	-	107,144,168,176	0
2	GHP	I	1	11/12	0.64	0.48	-	102,108,111,117	0
2	GHP	K	1	11/12	0.75	0.18	-	50,59,70,71	0
2	3FG	P	3	12/13	0.95	0.20	-	31,38,40,42	0
2	GHP	J	1	11/12	0.85	0.24	-	44,49,51,52	0
2	OMY	N	6	14/15	0.95	0.22	-	32,36,39,60	0
2	3FG	N	3	12/13	0.96	0.20	-	28,31,34,34	0
2	GHP	O	4	11/12	0.94	0.14	-	25,30,32,33	0
2	3MY	I	2	13/14	0.84	0.35	-	49,83,94,99	0
2	OMY	L	6	14/15	0.72	0.31	-	84,114,150,151	0
2	3FG	I	3	12/13	0.75	0.36	-	53,89,99,104	0
2	GHP	K	4	11/12	0.70	0.15	-	60,66,78,85	0
2	3MY	M	2	13/14	0.81	0.23	-	74,77,97,132	0
2	GHP	L	1	11/12	0.76	0.25	-	54,62,72,72	0
2	3FG	L	7	13/13	0.10	0.69	-	101,144,162,174	0
2	GHP	L	5	11/12	0.55	0.49	-	102,132,149,172	0
2	3FG	J	7	13/13	0.81	0.31	-	40,50,56,59	0
2	GHP	P	5	11/12	0.91	0.12	-	26,31,40,41	0
2	GHP	J	4	11/12	0.75	0.27	-	40,55,61,63	0
2	OMY	P	6	14/15	0.92	0.13	-	30,39,40,68	0
2	GHP	P	1	11/12	0.90	0.18	-	32,34,38,38	0
2	GHP	N	4	11/12	0.95	0.16	-	25,29,36,40	0
2	3FG	P	7	13/13	0.93	0.17	-	35,42,47,50	0
2	GHP	M	1	11/12	0.57	0.45	-	80,89,97,99	0
2	3FG	M	3	12/13	0.80	0.25	-	69,77,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	OMY	J	6	14/15	0.80	0.33	-	52,66,72,85	0
2	3FG	L	3	12/13	0.79	0.25	-	66,75,83,87	0

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^{th} 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^2)	Q<0.9
5	T55	P	101	11/12	0.75	0.36	14.45	33,41,78,79	0
4	CIT	B	603	13/13	0.88	0.20	10.70	38,56,71,78	0
4	CIT	C	602	13/13	0.92	0.27	9.04	45,55,62,67	0
5	T55	N	101	11/12	0.67	0.27	8.97	40,45,56,73	0
8	N1L	M	104	12/13	0.72	0.30	6.25	52,59,75,78	0
5	T55	B	602	11/12	0.75	0.43	5.90	48,50,65,72	0
6	MAN	P	102	11/12	0.92	0.20	5.85	28,39,50,57	0
4	CIT	D	602	13/13	0.93	0.23	5.70	39,43,51,54	0
4	CIT	A	602	13/13	0.85	0.19	5.47	37,46,55,59	0
7	NAG	M	103	14/15	0.47	0.92	5.36	108,139,149,151	0
5	T55	M	101	11/12	0.73	0.39	5.35	53,56,87,94	0
8	N1L	L	103	12/13	0.78	0.23	4.01	40,54,66,66	0
5	T55	K	101	11/12	0.78	0.30	3.76	51,56,62,71	0
7	NAG	L	102	14/15	0.69	0.62	2.83	107,135,149,153	0
8	N1L	K	104	12/13	0.83	0.20	2.73	36,56,70,73	0
7	NAG	K	103	14/15	0.44	0.77	2.22	107,133,142,154	0
7	NAG	N	103	14/15	0.94	0.15	1.25	30,40,45,48	0
3	FAD	C	601	53/53	0.97	0.13	0.33	19,22,28,32	0
3	FAD	A	601	53/53	0.99	0.10	-0.02	11,15,22,26	0
3	FAD	D	601	53/53	0.97	0.10	-0.15	20,26,38,43	0
3	FAD	B	601	53/53	0.98	0.10	-0.29	10,14,24,29	0
6	MAN	O	102	11/12	0.92	0.10	-0.82	34,40,45,49	0
6	MAN	N	102	11/12	0.92	0.21	-	38,45,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	N1L	O	104	12/13	0.88	0.24	-	33,40,48,55	0
6	MAN	M	102	11/12	0.50	0.72	-	112,144,153,160	0
6	MAN	K	102	11/12	0.43	0.76	-	136,145,157,161	0
4	CIT	O	105	13/13	0.88	0.21	-	31,40,50,51	0
8	N1L	N	104	12/13	0.88	0.30	-	40,42,50,50	0
6	MAN	J	101	11/12	0.79	0.27	-	52,62,67,77	0
7	NAG	P	103	14/15	0.86	0.16	-	40,45,48,54	0
6	MAN	I	101	11/12	0.09	1.04	-	103,132,139,141	0
7	NAG	I	102	14/15	0.56	0.49	-	71,83,106,107	0
7	NAG	J	102	14/15	0.63	0.43	-	81,93,113,114	0
8	N1L	P	104	12/13	0.93	0.22	-	29,32,37,51	0
5	T55	O	101	11/12	0.76	0.52	-	43,51,75,78	0
6	MAN	L	101	11/12	0.56	0.73	-	128,153,162,166	0
7	NAG	O	103	14/15	0.71	0.42	-	66,77,92,94	0

6.5 Other polymers (i)

There are no such residues in this entry.