



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:34 am GMT

PDB ID : 1TEI  
Title : STRUCTURE OF CONCAVALIN A COMPLEXED TO BETA-D-GLCNAC (1,2)ALPHA-D-MAN-(1,6)[BETA-D-GLCNAC(1,2)ALPHA-D-MAN (1,6)]ALPHA-D-MAN  
Authors : Naismith, J.H.; Moothoo, D.N.  
Deposited on : 1997-05-28  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

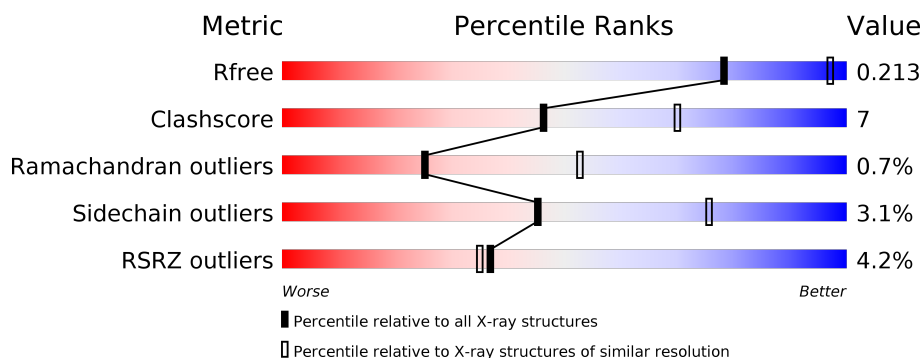
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	<div> <div>3%</div> <div>85%</div> <div>14%</div> </div>
1	B	237	<div> <div>3%</div> <div>84%</div> <div>14%</div> </div>
1	C	237	<div> <div>%</div> <div>83%</div> <div>14%</div> </div>
1	D	237	<div> <div>3%</div> <div>83%</div> <div>14%</div> </div>
1	E	237	<div> <div>5%</div> <div>82%</div> <div>16%</div> </div>
1	F	237	<div> <div>9%</div> <div>81%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	237	
1	H	237	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	F	243	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15060 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 CONCANAVALLIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	37	0	0
			1809	1141	302	364	2			
1	B	237	Total	C	N	O	S	45	0	0
			1809	1141	302	364	2			
1	C	237	Total	C	N	O	S	30	0	0
			1809	1141	302	364	2			
1	D	237	Total	C	N	O	S	62	0	0
			1809	1141	302	364	2			
1	E	237	Total	C	N	O	S	28	0	0
			1809	1141	302	364	2			
1	F	237	Total	C	N	O	S	78	0	0
			1809	1141	302	364	2			
1	G	237	Total	C	N	O	S	26	0	0
			1809	1141	302	364	2			
1	H	237	Total	C	N	O	S	64	0	0
			1809	1141	302	364	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	CONFLICT	UNP P02866
A	155	GLU	ARG	CONFLICT	UNP P02866
B	151	ASP	GLU	CONFLICT	UNP P02866
B	155	GLU	ARG	CONFLICT	UNP P02866
C	151	ASP	GLU	CONFLICT	UNP P02866
C	155	GLU	ARG	CONFLICT	UNP P02866
D	151	ASP	GLU	CONFLICT	UNP P02866
D	155	GLU	ARG	CONFLICT	UNP P02866
E	151	ASP	GLU	CONFLICT	UNP P02866
E	155	GLU	ARG	CONFLICT	UNP P02866
F	151	ASP	GLU	CONFLICT	UNP P02866
F	155	GLU	ARG	CONFLICT	UNP P02866
G	151	ASP	GLU	CONFLICT	UNP P02866

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Chain	Residue	Modelled	Actual	Comment	Reference
G	155	GLU	ARG	CONFLICT	UNP P02866
H	151	ASP	GLU	CONFLICT	UNP P02866
H	155	GLU	ARG	CONFLICT	UNP P02866

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			62	34	2	26		
2	B	5	Total	C	N	O	0	0
			62	34	2	26		
2	C	5	Total	C	N	O	0	0
			62	34	2	26		
2	D	5	Total	C	N	O	0	0
			62	34	2	26		
2	E	5	Total	C	N	O	0	0
			62	34	2	26		
2	F	5	Total	C	N	O	11	0
			62	34	2	26		
2	G	5	Total	C	N	O	0	0
			62	34	2	26		
2	H	5	Total	C	N	O	10	0
			62	34	2	26		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	E	1	Total 1	Ca 1	0	0
4	H	1	Total 1	Ca 1	0	0
4	B	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0

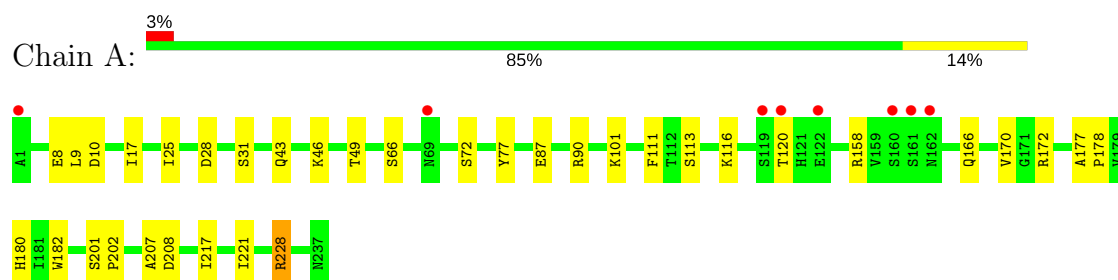
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0
5	B	10	Total 10	O 10	0	0
5	C	13	Total 13	O 13	0	0
5	D	7	Total 7	O 7	0	0
5	E	19	Total 19	O 19	0	0
5	F	5	Total 5	O 5	0	0
5	G	5	Total 5	O 5	0	0
5	H	2	Total 2	O 2	0	0

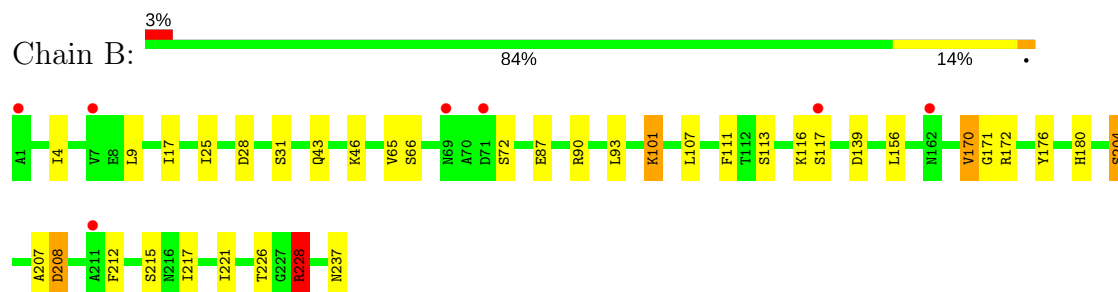
### 3 Residue-property plots [i](#)

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

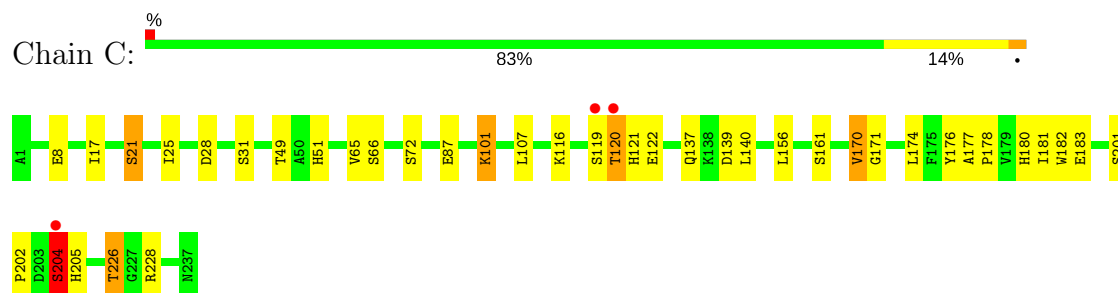
#### • Molecule 1: CONCANAVALIN A



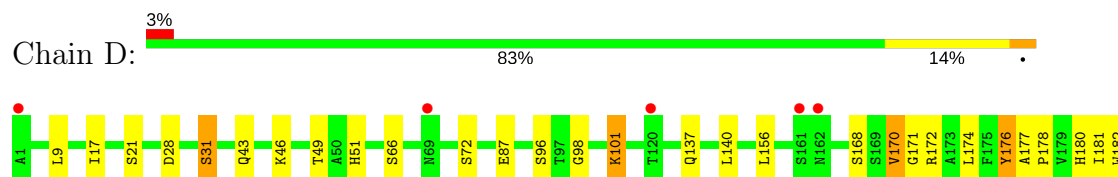
#### • Molecule 1: CONCANAVALIN A



#### • Molecule 1: CONCANAVALIN A

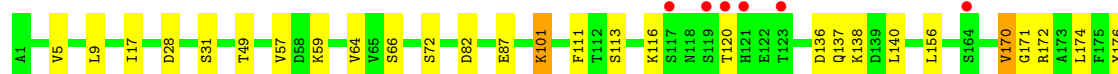
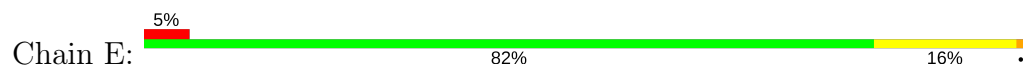


#### • Molecule 1: CONCANAVALIN A

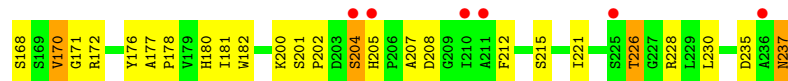
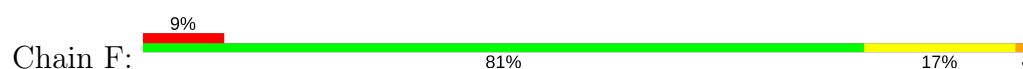




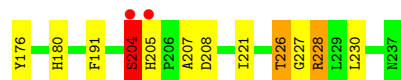
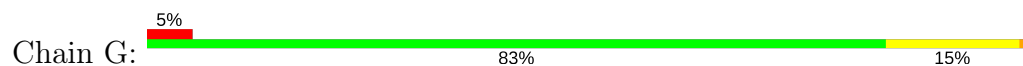
• Molecule 1: CONCAVALIN A



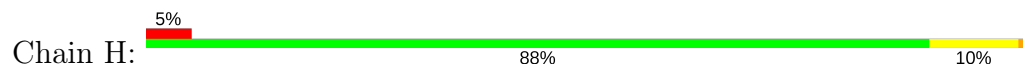
• Molecule 1: CONCAVALIN A



• Molecule 1: CONCAVALIN A



• Molecule 1: CONCAVALIN A





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.50Å 122.80Å 124.60Å 90.00° 134.20° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 24.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.00-2.70) 97.1 (24.51-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.09 (at 2.71Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.179 , 0.219 0.174 , 0.213	Depositor DCC
$R_{free}$ test set	5119 reflections (11.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.000 for k+l,h+l,-l 0.000 for -k+l,-h-l,-l 0.009 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.000 for h-k+l,l,-h-l 0.000 for -k-l,-h-l,k 0.000 for h+k+l,-l,-h-l 0.000 for k-l,h+l,-k 0.007 for h,-k,-h-l 0.021 for -h-2*k,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.55	0/1851	0.83	1/2522 (0.0%)
1	B	0.50	0/1851	0.78	1/2522 (0.0%)
1	C	0.53	0/1851	0.81	0/2522
1	D	0.57	1/1851 (0.1%)	0.81	1/2522 (0.0%)
1	E	0.54	0/1851	0.82	2/2522 (0.1%)
1	F	0.50	0/1851	0.79	1/2522 (0.0%)
1	G	0.51	0/1851	0.80	0/2522
1	H	0.54	1/1851 (0.1%)	0.79	0/2522
All	All	0.53	2/14808 (0.0%)	0.80	6/20176 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	176	TYR	CE2-CZ	-5.71	1.31	1.38
1	H	176	TYR	CE1-CZ	-5.28	1.31	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	LEU	N-CA-C	-5.17	97.03	111.00
1	F	9	LEU	N-CA-C	-5.17	97.05	111.00
1	A	9	LEU	N-CA-C	-5.15	97.11	111.00
1	B	9	LEU	N-CA-C	-5.08	97.28	111.00
1	D	9	LEU	N-CA-C	-5.06	97.34	111.00
1	E	5	VAL	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1755	26	1
1	B	1809	0	1755	23	0
1	C	1809	0	1755	30	0
1	D	1809	0	1755	28	0
1	E	1809	0	1755	32	0
1	F	1809	0	1755	28	0
1	G	1809	0	1755	37	0
1	H	1809	0	1755	24	0
2	A	62	0	54	1	0
2	B	62	0	54	1	0
2	C	62	0	54	1	0
2	D	62	0	54	2	0
2	E	62	0	54	1	0
2	F	62	0	54	1	1
2	G	62	0	54	1	0
2	H	62	0	54	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	15	0	0	2	0
5	B	10	0	0	2	0
5	C	13	0	0	1	0
5	D	7	0	0	0	0
5	E	19	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	5	0	0	1	0
5	G	5	0	0	0	0
5	H	2	0	0	0	0
All	All	15060	0	14472	206	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (206) 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:E:82:ASP:HB2	5:E:258:HOH:O	1.77	0.83
1:F:204:SER:HB2	1:F:205:HIS:CD2	2.16	0.79
1:F:207:ALA:HB1	1:F:208:ASP:OD2	1.83	0.79
1:C:17:ILE:HD13	1:C:228:ARG:HD3	1.65	0.79
1:F:170:VAL:HG22	1:F:226:THR:HG23	1.64	0.79
1:A:17:ILE:HD13	1:A:228:ARG:HD3	1.63	0.79
1:D:17:ILE:HD13	1:D:228:ARG:HD3	1.62	0.79
1:H:172:ARG:HD2	1:H:221:ILE:HG12	1.65	0.78
1:E:228:ARG:HG2	2:E:241:MAN:O3	1.84	0.78
1:E:49:THR:HG21	1:G:116:LYS:NZ	2.00	0.77
1:B:172:ARG:HD2	1:B:221:ILE:HG12	1.68	0.76
5:A:252:HOH:O	1:C:51:HIS:HB2	1.86	0.74
1:A:116:LYS:NZ	1:C:49:THR:HG21	2.03	0.73
1:G:17:ILE:HD13	1:G:228:ARG:HD3	1.71	0.73
1:A:116:LYS:HZ3	1:C:49:THR:HG21	1.53	0.71
5:F:247:HOH:O	1:H:51:HIS:HB2	1.90	0.71
1:F:204:SER:HB2	1:F:205:HIS:HD2	1.56	0.70
1:B:17:ILE:HD13	1:B:228:ARG:HD3	1.73	0.70
1:H:17:ILE:HD13	1:H:228:ARG:HD3	1.72	0.70
1:E:57:VAL:HG22	1:G:64:VAL:HG21	1.74	0.69
1:G:66:SER:HB3	1:G:72:SER:HB3	1.75	0.68
1:H:170:VAL:HG22	1:H:226:THR:HG22	1.75	0.68
1:G:228:ARG:HG2	2:G:241:MAN:O3	1.94	0.68
1:F:116:LYS:HZ1	1:H:49:THR:HG21	1.60	0.66
5:B:249:HOH:O	1:D:51:HIS:HB2	1.95	0.66
1:E:17:ILE:HD13	1:E:228:ARG:HD3	1.76	0.65
1:B:66:SER:HB3	1:B:72:SER:HB3	1.77	0.65
1:B:116:LYS:HZ1	1:D:49:THR:HG21	1.60	0.65
1:B:170:VAL:HG22	1:B:226:THR:HG22	1.77	0.65
1:C:66:SER:HB3	1:C:72:SER:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ARG:HG2	2:B:241:MAN:O3	1.97	0.64
1:F:205:HIS:CD2	1:F:205:HIS:N	2.66	0.64
1:C:228:ARG:HG2	2:C:241:MAN:O3	1.98	0.64
1:E:49:THR:HG21	1:G:116:LYS:HZ1	1.64	0.62
1:A:66:SER:HB3	1:A:72:SER:HB3	1.81	0.62
1:B:156:LEU:O	1:B:171:GLY:HA3	2.00	0.62
1:E:220:SER:HB2	5:E:255:HOH:O	2.00	0.60
1:H:172:ARG:HD2	1:H:221:ILE:CG1	2.30	0.60
1:B:172:ARG:HD2	1:B:221:ILE:CG1	2.31	0.60
1:D:228:ARG:HG2	2:D:241:MAN:O3	2.01	0.59
1:H:66:SER:HB3	1:H:72:SER:HB3	1.83	0.59
1:D:156:LEU:O	1:D:171:GLY:HA3	2.02	0.59
1:F:116:LYS:NZ	1:H:49:THR:HG21	2.17	0.58
1:C:178:PRO:HD3	1:D:176:TYR:HD1	1.69	0.58
1:D:172:ARG:HD2	1:D:221:ILE:HG12	1.85	0.58
1:E:49:THR:HG21	1:G:116:LYS:HZ3	1.68	0.57
1:E:59:LYS:HE3	5:E:256:HOH:O	2.03	0.56
1:E:204:SER:HB2	1:E:205:HIS:CD2	2.40	0.56
1:F:172:ARG:HD2	1:F:221:ILE:HG12	1.88	0.56
1:G:43:GLN:HE21	1:G:46:LYS:HD2	1.71	0.56
1:E:66:SER:HB3	1:E:72:SER:HB3	1.87	0.56
1:G:204:SER:HB2	1:G:205:HIS:CD2	2.41	0.55
1:F:156:LEU:O	1:F:171:GLY:HA3	2.05	0.55
1:G:156:LEU:O	1:G:171:GLY:HA3	2.07	0.55
1:F:28:ASP:HB3	1:F:31:SER:O	2.07	0.54
1:B:116:LYS:NZ	1:D:49:THR:HG21	2.23	0.54
1:A:43:GLN:HE21	1:A:46:LYS:HD2	1.73	0.54
1:D:170:VAL:HG22	1:D:226:THR:CG2	2.37	0.54
1:C:119:SER:HB2	1:C:122:GLU:HB2	1.90	0.54
1:F:43:GLN:HE21	1:F:46:LYS:HD2	1.72	0.54
1:E:116:LYS:NZ	1:G:49:THR:HG21	2.23	0.54
1:A:116:LYS:NZ	5:A:252:HOH:O	2.39	0.53
1:B:66:SER:HB3	1:B:72:SER:CB	2.38	0.53
1:A:49:THR:HG21	1:C:116:LYS:NZ	2.24	0.53
1:C:170:VAL:HG22	1:C:226:THR:CG2	2.39	0.53
1:H:101:LYS:N	1:H:101:LYS:HD3	2.24	0.52
1:E:156:LEU:O	1:E:171:GLY:HA3	2.09	0.52
1:A:87:GLU:HG3	1:A:182:TRP:O	2.09	0.52
1:G:176:TYR:CE2	1:H:176:TYR:HE1	2.28	0.52
1:E:101:LYS:N	1:E:101:LYS:HD3	2.24	0.52
1:H:228:ARG:HG2	2:H:241:MAN:O3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:SER:HB2	1:C:205:HIS:CD2	2.45	0.51
1:D:66:SER:HB3	1:D:72:SER:HB3	1.92	0.51
1:A:228:ARG:HG2	2:A:241:MAN:O3	2.10	0.51
1:H:181:ILE:HG23	1:H:182:TRP:HD1	1.75	0.51
1:A:66:SER:HB3	1:A:72:SER:CB	2.40	0.51
1:D:170:VAL:HG22	1:D:226:THR:HG22	1.91	0.51
1:E:235:ASP:OD1	1:E:237:ASN:HB2	2.11	0.50
1:B:111:PHE:CE2	1:B:113:SER:HB2	2.47	0.50
1:F:66:SER:HB3	1:F:72:SER:HB3	1.93	0.50
1:B:43:GLN:HE21	1:B:46:LYS:HD2	1.76	0.50
1:G:66:SER:HB3	1:G:72:SER:CB	2.41	0.50
1:G:101:LYS:HD3	1:G:101:LYS:N	2.26	0.50
1:G:172:ARG:HD2	1:G:221:ILE:CG1	2.41	0.50
1:C:181:ILE:HG23	1:C:182:TRP:HD1	1.77	0.50
1:D:43:GLN:HE21	1:D:46:LYS:HD2	1.77	0.50
1:C:87:GLU:HG2	1:C:180:HIS:NE2	2.27	0.49
1:H:170:VAL:HG22	1:H:226:THR:CG2	2.41	0.49
1:E:172:ARG:HD2	1:E:221:ILE:HG12	1.94	0.49
1:D:101:LYS:N	1:D:101:LYS:HD3	2.27	0.49
1:C:28:ASP:HB3	1:C:31:SER:O	2.11	0.49
1:C:178:PRO:HD3	1:D:176:TYR:CD1	2.47	0.49
1:A:158:ARG:HG3	1:A:166:GLN:HG3	1.94	0.49
1:H:87:GLU:HG2	1:H:180:HIS:NE2	2.28	0.48
1:D:181:ILE:HG23	1:D:182:TRP:HD1	1.78	0.48
1:F:172:ARG:HD2	1:F:221:ILE:CG1	2.44	0.48
1:G:208:ASP:OD1	1:G:227:GLY:HA2	2.13	0.48
1:A:172:ARG:HD2	1:A:221:ILE:HG12	1.94	0.47
1:H:156:LEU:O	1:H:171:GLY:HA3	2.13	0.47
1:G:87:GLU:HG2	1:G:180:HIS:NE2	2.29	0.47
1:H:204:SER:HB2	1:H:205:HIS:CD2	2.49	0.47
1:B:25:ILE:HG21	1:B:65:VAL:HG21	1.97	0.47
1:A:17:ILE:CD1	1:A:228:ARG:HD3	2.41	0.47
1:E:176:TYR:CE2	1:F:176:TYR:CE2	3.02	0.47
1:E:64:VAL:HG21	1:G:57:VAL:HG22	1.97	0.47
1:B:17:ILE:CD1	1:B:228:ARG:HD3	2.42	0.47
1:G:43:GLN:NE2	1:G:46:LYS:HD2	2.30	0.47
1:E:170:VAL:HG22	1:E:226:THR:HG22	1.97	0.47
1:H:170:VAL:HG13	1:H:226:THR:HA	1.95	0.47
1:C:25:ILE:HG21	1:C:65:VAL:HG21	1.96	0.46
1:A:116:LYS:HZ3	1:C:49:THR:CG2	2.25	0.46
1:H:43:GLN:HE21	1:H:46:LYS:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLN:HG2	1:C:140:LEU:HD12	1.96	0.46
1:D:137:GLN:HG2	1:D:140:LEU:HD12	1.96	0.46
1:H:8:GLU:O	1:H:25:ILE:HA	2.16	0.46
1:D:181:ILE:HG23	1:D:182:TRP:CD1	2.51	0.46
1:D:96:SER:OG	1:D:230:LEU:HA	2.16	0.46
1:G:150:THR:O	1:G:151:ASP:HB2	2.15	0.46
1:C:87:GLU:HG2	1:C:180:HIS:CD2	2.50	0.46
1:E:174:LEU:N	1:E:174:LEU:HD12	2.31	0.46
1:E:111:PHE:CE2	1:E:113:SER:HB2	2.51	0.46
1:E:87:GLU:HG3	1:E:182:TRP:O	2.14	0.46
1:B:139:ASP:O	1:B:176:TYR:HB2	2.16	0.46
1:E:28:ASP:HB3	1:E:31:SER:O	2.16	0.46
1:C:170:VAL:HG22	1:C:226:THR:HG22	1.98	0.45
1:G:8:GLU:O	1:G:25:ILE:HA	2.16	0.45
1:C:177:ALA:HA	1:C:178:PRO:HD3	1.87	0.45
1:F:96:SER:OG	1:F:230:LEU:HA	2.17	0.45
1:B:107:LEU:N	1:B:107:LEU:HD12	2.32	0.45
1:E:87:GLU:HG2	1:E:180:HIS:CD2	2.52	0.45
1:D:98:GLY:HA2	2:D:240:NAG:O7	2.17	0.45
1:F:205:HIS:HD2	1:F:205:HIS:N	2.13	0.45
1:G:172:ARG:HD2	1:G:221:ILE:HG12	1.98	0.45
1:C:8:GLU:O	1:C:25:ILE:HA	2.17	0.45
1:G:176:TYR:CE2	1:H:176:TYR:CE1	3.05	0.45
1:C:156:LEU:O	1:C:171:GLY:HA3	2.18	0.44
1:E:116:LYS:HZ1	1:G:49:THR:HG21	1.80	0.44
1:G:96:SER:OG	1:G:230:LEU:HA	2.17	0.44
1:A:177:ALA:HA	1:A:178:PRO:HD3	1.83	0.44
1:H:87:GLU:HG2	1:H:180:HIS:CD2	2.52	0.44
1:A:172:ARG:HD2	1:A:221:ILE:CG1	2.47	0.44
1:A:87:GLU:HG2	1:A:180:HIS:CD2	2.52	0.44
1:E:87:GLU:HG2	1:E:180:HIS:NE2	2.32	0.44
1:A:90:ARG:NH1	1:A:217:ILE:HG23	2.32	0.44
1:D:17:ILE:CD1	1:D:228:ARG:HD3	2.41	0.44
1:F:87:GLU:HG2	1:F:180:HIS:CD2	2.53	0.44
1:D:28:ASP:HB3	1:D:31:SER:O	2.17	0.44
1:D:201:SER:HA	1:D:202:PRO:HD3	1.86	0.44
1:G:170:VAL:HG22	1:G:226:THR:CG2	2.48	0.44
1:E:207:ALA:HA	1:E:208:ASP:HA	1.81	0.43
1:E:64:VAL:HG21	1:G:57:VAL:CG2	2.48	0.43
1:B:93:LEU:HD23	1:B:212:PHE:HA	2.00	0.43
1:E:136:ASP:OD2	1:E:138:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:GLN:NE2	1:F:46:LYS:HD2	2.33	0.43
1:D:208:ASP:OD1	1:D:227:GLY:HA2	2.18	0.43
1:F:111:PHE:CE2	1:F:113:SER:HB2	2.54	0.43
1:B:87:GLU:HG2	1:B:180:HIS:NE2	2.34	0.43
1:C:183:GLU:HG2	5:C:256:HOH:O	2.17	0.43
1:E:210:ILE:HG22	1:E:211:ALA:N	2.34	0.43
1:C:174:LEU:HD12	1:C:174:LEU:N	2.34	0.43
1:F:200:LYS:HE3	1:F:200:LYS:HB2	1.88	0.42
1:A:43:GLN:NE2	1:A:46:LYS:HD2	2.34	0.42
1:A:87:GLU:HG2	1:A:180:HIS:NE2	2.34	0.42
1:C:120:THR:O	1:C:122:GLU:N	2.52	0.42
1:E:137:GLN:HG2	1:E:140:LEU:HD12	2.02	0.42
1:F:201:SER:HA	1:F:202:PRO:HD3	1.84	0.42
1:F:235:ASP:OD1	1:F:237:ASN:HB3	2.18	0.42
1:G:174:LEU:HD12	1:G:174:LEU:N	2.34	0.42
1:B:90:ARG:NH1	1:B:217:ILE:HG23	2.34	0.42
1:A:28:ASP:HB3	1:A:31:SER:O	2.18	0.42
1:B:207:ALA:HA	1:B:208:ASP:HA	1.82	0.42
1:D:174:LEU:N	1:D:174:LEU:HD12	2.34	0.42
1:F:177:ALA:HA	1:F:178:PRO:HD3	1.86	0.42
1:G:119:SER:O	1:G:122:GLU:HB2	2.20	0.42
1:B:101:LYS:HD3	1:B:101:LYS:N	2.35	0.42
1:G:87:GLU:HG2	1:G:180:HIS:CD2	2.55	0.42
1:B:28:ASP:HB3	1:B:31:SER:O	2.20	0.42
1:D:87:GLU:HG2	1:D:180:HIS:CD2	2.54	0.42
1:F:168:SER:HG	2:F:240:NAG:C7	2.33	0.42
1:F:14:ASN:C	1:F:19:ASP:HB2	2.40	0.42
1:H:181:ILE:HG23	1:H:182:TRP:CD1	2.52	0.42
1:A:111:PHE:CE2	1:A:113:SER:HB2	2.54	0.42
1:C:107:LEU:HD12	1:C:107:LEU:N	2.35	0.42
1:F:4:ILE:HD13	1:F:215:SER:HB3	2.02	0.42
1:G:117:SER:HB3	1:G:118:ASN:H	1.68	0.42
1:E:57:VAL:HG13	1:G:64:VAL:HG22	2.02	0.42
1:A:201:SER:HA	1:A:202:PRO:HD3	1.83	0.41
1:C:139:ASP:O	1:C:176:TYR:HB2	2.20	0.41
1:B:4:ILE:HD13	1:B:215:SER:HB3	2.01	0.41
1:G:43:GLN:NE2	1:G:46:LYS:NZ	2.68	0.41
5:B:249:HOH:O	1:D:51:HIS:CG	2.73	0.41
1:G:170:VAL:HG22	1:G:226:THR:HG23	2.01	0.41
1:G:112:THR:O	1:G:191:PHE:HA	2.21	0.41
1:C:101:LYS:HD3	1:C:101:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:SER:HA	1:C:202:PRO:HD3	1.87	0.41
1:D:237:ASN:HA	1:D:237:ASN:HD22	1.64	0.41
1:G:28:ASP:HB3	1:G:31:SER:O	2.20	0.41
1:H:87:GLU:HG3	1:H:182:TRP:O	2.20	0.41
1:F:181:ILE:HG23	1:F:182:TRP:HD1	1.85	0.41
1:A:207:ALA:HA	1:A:208:ASP:HA	1.83	0.41
1:A:8:GLU:O	1:A:25:ILE:HA	2.20	0.40
1:A:8:GLU:OE2	1:A:10:ASP:HB2	2.21	0.40
1:H:177:ALA:HA	1:H:178:PRO:HD3	1.91	0.40
1:D:177:ALA:HA	1:D:178:PRO:HD3	1.92	0.40
1:F:93:LEU:HD23	1:F:212:PHE:HA	2.03	0.40
1:G:207:ALA:HA	1:G:208:ASP:HA	1.80	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:OH	2:F:244:NAG:O7[3_445]	2.11	0.09

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/237 (99%)	220 (94%)	14 (6%)	1 (0%)	38	66
1	B	235/237 (99%)	219 (93%)	14 (6%)	2 (1%)	20	46
1	C	235/237 (99%)	221 (94%)	11 (5%)	3 (1%)	14	35
1	D	235/237 (99%)	220 (94%)	14 (6%)	1 (0%)	38	66
1	E	235/237 (99%)	215 (92%)	19 (8%)	1 (0%)	38	66
1	F	235/237 (99%)	218 (93%)	15 (6%)	2 (1%)	20	46
1	G	235/237 (99%)	216 (92%)	17 (7%)	2 (1%)	20	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	235/237 (99%)	216 (92%)	17 (7%)	2 (1%)	20	46
All	All	1880/1896 (99%)	1745 (93%)	121 (6%)	14 (1%)	25	53

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	204	SER
1	H	150	THR
1	B	204	SER
1	B	228	ARG
1	C	121	HIS
1	D	204	SER
1	E	228	ARG
1	G	150	THR
1	G	204	SER
1	H	228	ARG
1	C	21	SER
1	F	228	ARG
1	A	228	ARG
1	C	204	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/203 (100%)	200 (98%)	3 (2%)	70	90
1	B	203/203 (100%)	196 (97%)	7 (3%)	42	73
1	C	203/203 (100%)	196 (97%)	7 (3%)	42	73
1	D	203/203 (100%)	194 (96%)	9 (4%)	33	63
1	E	203/203 (100%)	197 (97%)	6 (3%)	46	76
1	F	203/203 (100%)	197 (97%)	6 (3%)	46	76
1	G	203/203 (100%)	197 (97%)	6 (3%)	46	76
1	H	203/203 (100%)	197 (97%)	6 (3%)	46	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1624/1624 (100%)	1574 (97%)	50 (3%)	45 75

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	120	THR
1	A	170	VAL
1	B	101	LYS
1	B	117	SER
1	B	170	VAL
1	B	204	SER
1	B	208	ASP
1	B	228	ARG
1	B	237	ASN
1	C	21	SER
1	C	101	LYS
1	C	120	THR
1	C	161	SER
1	C	170	VAL
1	C	204	SER
1	C	226	THR
1	D	21	SER
1	D	31	SER
1	D	101	LYS
1	D	168	SER
1	D	170	VAL
1	D	185	SER
1	D	204	SER
1	D	228	ARG
1	D	237	ASN
1	E	101	LYS
1	E	120	THR
1	E	170	VAL
1	E	204	SER
1	E	223	SER
1	E	228	ARG
1	F	101	LYS
1	F	120	THR
1	F	161	SER
1	F	170	VAL
1	F	226	THR

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Mol	Chain	Res	Type
1	F	237	ASN
1	G	101	LYS
1	G	120	THR
1	G	170	VAL
1	G	204	SER
1	G	226	THR
1	G	228	ARG
1	H	101	LYS
1	H	158	ARG
1	H	168	SER
1	H	170	VAL
1	H	204	SER
1	H	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	237	ASN
1	B	43	GLN
1	B	205	HIS
1	B	237	ASN
1	C	166	GLN
1	C	205	HIS
1	C	237	ASN
1	D	43	GLN
1	D	237	ASN
1	E	205	HIS
1	E	237	ASN
1	F	43	GLN
1	F	205	HIS
1	F	237	ASN
1	G	43	GLN
1	G	69	ASN
1	G	205	HIS
1	G	237	ASN
1	H	43	GLN
1	H	205	HIS
1	H	237	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

40 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	240	2	14,14,15	0.49	0	15,19,21	1.10	2 (13%)
2	MAN	A	241	2	11,11,12	0.53	0	13,15,17	0.49	0
2	MAN	A	242	2	12,12,12	0.53	0	17,17,17	0.74	1 (5%)
2	MAN	A	243	2	11,11,12	0.40	0	13,15,17	0.88	0
2	NAG	A	244	2	14,14,15	0.52	0	15,19,21	0.90	1 (6%)
2	NAG	B	240	2	14,14,15	0.38	0	15,19,21	1.01	0
2	MAN	B	241	2	11,11,12	0.32	0	13,15,17	0.65	0
2	MAN	B	242	2	12,12,12	0.45	0	17,17,17	0.75	0
2	MAN	B	243	2	11,11,12	0.55	0	13,15,17	0.64	0
2	NAG	B	244	2	14,14,15	0.59	0	15,19,21	0.90	1 (6%)
2	NAG	C	240	2	14,14,15	0.41	0	15,19,21	1.08	0
2	MAN	C	241	2	11,11,12	0.55	0	13,15,17	0.41	0
2	MAN	C	242	2	12,12,12	0.32	0	17,17,17	0.72	0
2	MAN	C	243	2	11,11,12	0.65	0	13,15,17	0.49	0
2	NAG	C	244	2	14,14,15	0.47	0	15,19,21	0.99	1 (6%)
2	NAG	D	240	2	14,14,15	0.43	0	15,19,21	0.90	0
2	MAN	D	241	2	11,11,12	0.28	0	13,15,17	0.56	0
2	MAN	D	242	2	12,12,12	0.50	0	17,17,17	0.69	0
2	MAN	D	243	2	11,11,12	0.45	0	13,15,17	0.69	0
2	NAG	D	244	2	14,14,15	0.54	0	15,19,21	1.13	2 (13%)
2	NAG	E	240	2	14,14,15	0.45	0	15,19,21	1.14	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	E	241	2	11,11,12	0.41	0	13,15,17	0.49	0
2	MAN	E	242	2	12,12,12	0.39	0	17,17,17	0.64	0
2	MAN	E	243	2	11,11,12	0.40	0	13,15,17	0.75	0
2	NAG	E	244	2	14,14,15	0.36	0	15,19,21	0.86	1 (6%)
2	NAG	F	240	2	14,14,15	0.58	0	15,19,21	1.03	0
2	MAN	F	241	2	11,11,12	0.39	0	13,15,17	0.56	0
2	MAN	F	242	2	12,12,12	0.42	0	17,17,17	0.73	0
2	MAN	F	243	2	11,11,12	0.72	0	13,15,17	0.62	0
2	NAG	F	244	2	14,14,15	0.58	0	15,19,21	1.07	2 (13%)
2	NAG	G	240	2	14,14,15	0.38	0	15,19,21	1.11	1 (6%)
2	MAN	G	241	2	11,11,12	0.39	0	13,15,17	0.55	0
2	MAN	G	242	2	12,12,12	0.49	0	17,17,17	0.69	0
2	MAN	G	243	2	11,11,12	0.45	0	13,15,17	0.80	0
2	NAG	G	244	2	14,14,15	0.49	0	15,19,21	0.64	0
2	NAG	H	240	2	14,14,15	0.64	0	15,19,21	0.77	0
2	MAN	H	241	2	11,11,12	0.54	0	13,15,17	0.61	0
2	MAN	H	242	2	12,12,12	0.52	0	17,17,17	0.67	0
2	MAN	H	243	2	11,11,12	0.48	0	13,15,17	0.87	0
2	NAG	H	244	2	14,14,15	0.77	1 (7%)	15,19,21	0.82	1 (6%)

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	NAG	A	240	2	-	0/6/23/26	0/1/1/1
2	MAN	A	241	2	-	0/2/19/22	0/1/1/1
2	MAN	A	242	2	-	0/2/22/22	0/1/1/1
2	MAN	A	243	2	-	0/2/19/22	0/1/1/1
2	NAG	A	244	2	-	0/6/23/26	0/1/1/1
2	NAG	B	240	2	-	0/6/23/26	0/1/1/1
2	MAN	B	241	2	-	0/2/19/22	0/1/1/1
2	MAN	B	242	2	-	0/2/22/22	0/1/1/1
2	MAN	B	243	2	-	0/2/19/22	0/1/1/1
2	NAG	B	244	2	-	0/6/23/26	0/1/1/1
2	NAG	C	240	2	-	0/6/23/26	0/1/1/1
2	MAN	C	241	2	-	0/2/19/22	0/1/1/1
2	MAN	C	242	2	-	0/2/22/22	0/1/1/1
2	MAN	C	243	2	-	0/2/19/22	0/1/1/1
2	NAG	C	244	2	-	0/6/23/26	0/1/1/1
2	NAG	D	240	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	D	241	2	-	0/2/19/22	0/1/1/1
2	MAN	D	242	2	-	0/2/22/22	0/1/1/1
2	MAN	D	243	2	-	0/2/19/22	0/1/1/1
2	NAG	D	244	2	-	0/6/23/26	0/1/1/1
2	NAG	E	240	2	-	0/6/23/26	0/1/1/1
2	MAN	E	241	2	-	0/2/19/22	0/1/1/1
2	MAN	E	242	2	-	0/2/22/22	0/1/1/1
2	MAN	E	243	2	-	0/2/19/22	0/1/1/1
2	NAG	E	244	2	-	0/6/23/26	0/1/1/1
2	NAG	F	240	2	-	0/6/23/26	0/1/1/1
2	MAN	F	241	2	-	0/2/19/22	0/1/1/1
2	MAN	F	242	2	-	0/2/22/22	0/1/1/1
2	MAN	F	243	2	-	0/2/19/22	0/1/1/1
2	NAG	F	244	2	-	0/6/23/26	0/1/1/1
2	NAG	G	240	2	-	0/6/23/26	0/1/1/1
2	MAN	G	241	2	-	0/2/19/22	0/1/1/1
2	MAN	G	242	2	-	0/2/22/22	0/1/1/1
2	MAN	G	243	2	-	0/2/19/22	0/1/1/1
2	NAG	G	244	2	-	0/6/23/26	0/1/1/1
2	NAG	H	240	2	-	0/6/23/26	0/1/1/1
2	MAN	H	241	2	-	0/2/19/22	0/1/1/1
2	MAN	H	242	2	-	0/2/22/22	0/1/1/1
2	MAN	H	243	2	-	0/2/19/22	0/1/1/1
2	NAG	H	244	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	244	NAG	C1-C2	2.26	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	240	NAG	C3-C4-C5	-2.45	105.90	110.22
2	A	240	NAG	C1-C2-N2	-2.43	106.34	110.49
2	E	240	NAG	C3-C4-C5	-2.35	106.08	110.22
2	F	244	NAG	C2-N2-C7	-2.26	119.65	122.94
2	D	244	NAG	C2-N2-C7	-2.11	119.86	122.94
2	A	242	MAN	C6-C5-C4	-2.00	108.32	113.00
2	H	244	NAG	C1-O5-C5	2.00	114.93	112.17
2	F	244	NAG	C1-O5-C5	2.08	115.03	112.17
2	A	244	NAG	C1-O5-C5	2.08	115.03	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	244	NAG	C1-O5-C5	2.19	115.19	112.17
2	A	240	NAG	C6-C5-C4	2.34	118.47	113.00
2	E	240	NAG	C6-C5-C4	2.64	119.18	113.00
2	C	244	NAG	C1-O5-C5	2.68	115.86	112.17
2	B	244	NAG	C1-O5-C5	2.82	116.05	112.17
2	D	244	NAG	C1-O5-C5	3.18	116.55	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	241	MAN	1	0
2	B	241	MAN	1	0
2	C	241	MAN	1	0
2	D	240	NAG	1	0
2	D	241	MAN	1	0
2	E	241	MAN	1	0
2	F	240	NAG	1	0
2	F	244	NAG	0	1
2	G	241	MAN	1	0
2	H	241	MAN	1	0

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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	235/237 (99%)	-0.29	8 (3%)	46	45	6, 21, 49, 83	5 (2%)
1	B	232/237 (97%)	-0.23	7 (3%)	51	50	8, 27, 54, 70	3 (1%)
1	C	235/237 (99%)	-0.35	3 (1%)	77	78	6, 24, 55, 91	3 (1%)
1	D	233/237 (98%)	-0.18	6 (2%)	56	56	9, 26, 52, 68	7 (3%)
1	E	236/237 (99%)	-0.17	11 (4%)	32	30	7, 23, 54, 87	5 (2%)
1	F	234/237 (98%)	0.18	21 (8%)	10	8	13, 34, 61, 84	11 (4%)
1	G	237/237 (100%)	-0.13	12 (5%)	29	27	9, 27, 55, 70	5 (2%)
1	H	232/237 (97%)	0.13	11 (4%)	32	30	10, 32, 58, 73	8 (3%)
All	All	1874/1896 (98%)	-0.13	79 (4%)	37	35	6, 27, 56, 91	47 (2%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	121	HIS	9.6
1	F	120	THR	9.5
1	C	120	THR	9.2
1	E	120	THR	8.3
1	G	120	THR	7.3
1	A	120	THR	7.2
1	E	121	HIS	6.0
1	F	150	THR	5.1
1	B	1	ALA	4.8
1	E	185	SER	4.7
1	A	1	ALA	4.6
1	F	98	GLY	4.5
1	A	122	GLU	4.2
1	H	122	GLU	4.1
1	E	119	SER	4.0
1	G	69	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	120	THR	3.9
1	D	204	SER	3.9
1	E	187	VAL	3.8
1	F	163	GLY	3.7
1	F	205	HIS	3.7
1	F	69	ASN	3.6
1	F	161	SER	3.5
1	H	69	ASN	3.5
1	H	162	ASN	3.4
1	F	162	ASN	3.2
1	F	71	ASP	3.1
1	H	160	SER	3.0
1	G	150	THR	3.0
1	F	204	SER	3.0
1	H	21	SER	2.9
1	C	119	SER	2.9
1	D	161	SER	2.9
1	G	161	SER	2.9
1	E	117	SER	2.8
1	G	205	HIS	2.7
1	A	69	ASN	2.7
1	C	204	SER	2.7
1	H	71	ASP	2.6
1	H	185	SER	2.6
1	D	69	ASN	2.6
1	G	1	ALA	2.6
1	F	160	SER	2.6
1	A	119	SER	2.6
1	G	70	ALA	2.5
1	B	7	VAL	2.5
1	B	71	ASP	2.5
1	B	162	ASN	2.5
1	A	160	SER	2.5
1	B	211	ALA	2.4
1	F	9	LEU	2.4
1	H	83	ASN	2.4
1	H	211	ALA	2.4
1	H	13	PRO	2.3
1	D	1	ALA	2.3
1	A	162	ASN	2.3
1	E	188	VAL	2.3
1	F	236	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	160	SER	2.3
1	F	68	PRO	2.2
1	A	161	SER	2.2
1	F	166	GLN	2.2
1	H	16	ASP	2.2
1	E	204	SER	2.2
1	G	162	ASN	2.2
1	E	164	SER	2.2
1	E	123	THR	2.2
1	D	162	ASN	2.1
1	F	39	LYS	2.1
1	F	164	SER	2.1
1	F	210	ILE	2.1
1	G	119	SER	2.1
1	B	69	ASN	2.1
1	F	41	ASN	2.1
1	E	186	ALA	2.1
1	G	204	SER	2.1
1	B	117	SER	2.1
1	F	225	SER	2.1
1	F	211	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	F	243	11/12	0.71	0.32	4.20	23,27,31,32	0
2	NAG	B	244	14/15	0.88	0.23	1.56	41,45,50,53	0
2	MAN	F	242	12/12	0.84	0.27	1.21	47,50,53,56	0
2	MAN	G	242	12/12	0.93	0.22	1.00	34,39,44,47	0
2	NAG	E	244	14/15	0.91	0.18	0.99	33,37,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	H	240	14/15	0.91	0.25	0.94	29,35,50,50	0
2	NAG	F	244	14/15	0.81	0.30	0.73	22,28,31,32	11
2	NAG	F	240	14/15	0.88	0.28	0.42	35,42,48,52	0
2	NAG	G	240	14/15	0.94	0.14	0.27	26,30,35,36	0
2	NAG	C	240	14/15	0.95	0.15	0.26	20,23,33,41	0
2	MAN	B	241	11/12	0.95	0.16	0.22	27,32,36,40	0
2	NAG	A	240	14/15	0.97	0.14	0.19	14,19,27,28	0
2	MAN	H	241	11/12	0.89	0.22	0.07	36,41,46,49	0
2	NAG	E	240	14/15	0.96	0.13	0.06	11,16,21,22	0
2	NAG	B	240	14/15	0.94	0.17	0.03	23,30,38,38	0
2	MAN	F	241	11/12	0.87	0.20	-0.34	37,41,46,48	0
2	MAN	B	242	12/12	0.92	0.16	-0.37	35,39,45,46	0
2	NAG	D	240	14/15	0.95	0.14	-0.49	19,22,32,34	0
2	MAN	B	243	11/12	0.95	0.13	-0.70	34,35,38,44	0
2	NAG	A	244	14/15	0.94	0.12	-0.76	26,32,35,35	0
2	MAN	G	241	11/12	0.94	0.13	-0.87	25,31,32,33	0
2	MAN	A	241	11/12	0.99	0.10	-1.08	4,12,17,20	0
2	MAN	C	241	11/12	0.98	0.11	-1.42	19,24,25,25	0
2	MAN	A	242	12/12	0.96	0.09	-1.60	16,26,29,29	0
2	MAN	D	242	12/12	0.93	0.15	-1.64	37,38,40,46	0
2	MAN	E	242	12/12	0.96	0.11	-1.71	27,28,32,33	0
2	MAN	D	241	11/12	0.97	0.09	-2.21	19,24,27,29	0
2	MAN	E	241	11/12	0.96	0.10	-2.25	21,23,26,27	0
2	MAN	C	242	12/12	0.96	0.13	-2.58	32,35,36,39	0
2	MAN	G	243	11/12	0.94	0.27	-	41,43,48,54	0
2	MAN	A	243	11/12	0.96	0.12	-	17,18,23,36	0
2	MAN	D	243	11/12	0.94	0.17	-	30,35,41,47	0
2	MAN	C	243	11/12	0.93	0.19	-	42,44,47,52	0
2	NAG	D	244	14/15	0.83	0.27	-	46,51,55,56	0
2	MAN	E	243	11/12	0.95	0.15	-	24,26,32,39	0
2	NAG	G	244	14/15	0.85	0.37	-	51,54,60,63	0
2	NAG	H	244	14/15	0.49	0.25	-	59,64,65,66	10
2	NAG	C	244	14/15	0.88	0.30	-	47,49,51,51	0
2	MAN	H	242	12/12	0.86	0.30	-	46,49,55,55	0
2	MAN	H	243	11/12	0.83	0.36	-	53,55,58,62	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	F	239	1/1	0.72	0.18	-0.23	52,52,52,52	0
4	CA	D	239	1/1	0.94	0.16	-0.24	33,33,33,33	0
4	CA	C	239	1/1	0.97	0.12	-1.01	22,22,22,22	0
4	CA	G	239	1/1	0.97	0.12	-1.17	31,31,31,31	0
4	CA	H	246	1/1	0.77	0.11	-1.28	47,47,47,47	0
3	MN	H	245	1/1	0.93	0.11	-1.43	42,42,42,42	0
3	MN	C	238	1/1	0.99	0.08	-1.48	24,24,24,24	0
3	MN	B	238	1/1	0.99	0.04	-1.59	24,24,24,24	0
3	MN	E	238	1/1	0.99	0.09	-1.69	24,24,24,24	0
3	MN	A	238	1/1	0.99	0.09	-1.82	28,28,28,28	0
3	MN	G	238	1/1	0.99	0.07	-2.03	32,32,32,32	0
4	CA	A	239	1/1	0.94	0.09	-2.09	18,18,18,18	0
4	CA	B	239	1/1	0.97	0.06	-2.54	27,27,27,27	0
3	MN	D	238	1/1	0.98	0.06	-2.56	32,32,32,32	0
3	MN	F	238	1/1	0.97	0.03	-3.41	50,50,50,50	0
4	CA	E	239	1/1	0.99	0.07	-3.81	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.