



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 07:49 am GMT

PDB ID : 3Q0T  
Title : Crystal structure of human dpp-iv in complex withsa-(+)- methyl2-(3-(amino methyl)-4-(2,4-dichlorophenyl)-2-methyl- 7-oxo-5h-pyrrolo[3,4-b]pyridin-6(7h)-yl)acetate  
Authors : Klei, H.E.  
Deposited on : 2010-12-16  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

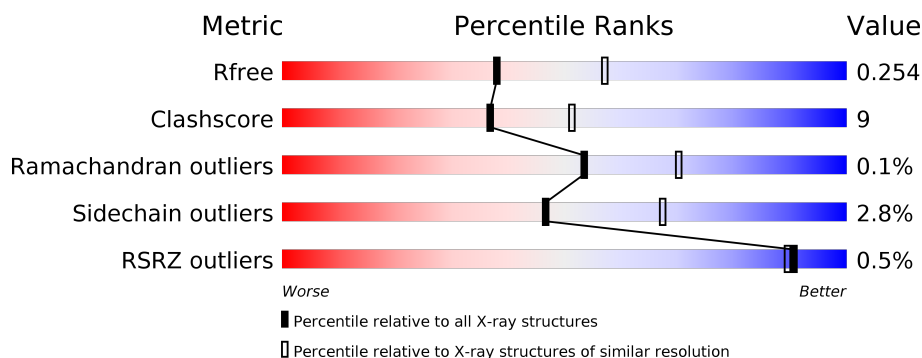
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	753	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 76%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> </div> <div>76% 20% ..</div> </div>
1	B	753	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 17%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> </div> <div>78% 17% ..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1501	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12467 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5896	3796	958	1116	26			
1	B	727	Total	C	N	O	S	0	0	0
			5892	3792	956	1118	26			

There are 50 discrepancies between the modelled and reference sequences:

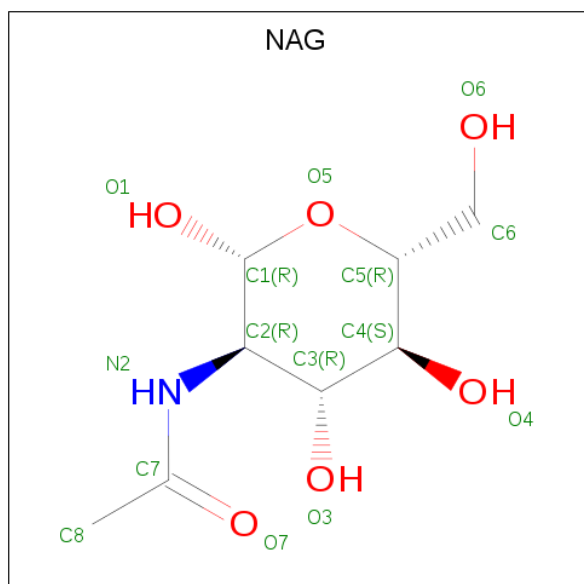
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLU	-	EXPRESSION TAG	UNP P27487
A	38	PHE	-	EXPRESSION TAG	UNP P27487
A	767	PRO	-	EXPRESSION TAG	UNP P27487
A	768	LEU	-	EXPRESSION TAG	UNP P27487
A	769	GLU	-	EXPRESSION TAG	UNP P27487
A	770	GLN	-	EXPRESSION TAG	UNP P27487
A	771	LYS	-	EXPRESSION TAG	UNP P27487
A	772	LEU	-	EXPRESSION TAG	UNP P27487
A	773	ILE	-	EXPRESSION TAG	UNP P27487
A	774	SER	-	EXPRESSION TAG	UNP P27487
A	775	GLU	-	EXPRESSION TAG	UNP P27487
A	776	GLU	-	EXPRESSION TAG	UNP P27487
A	777	ASP	-	EXPRESSION TAG	UNP P27487
A	778	LEU	-	EXPRESSION TAG	UNP P27487
A	779	ASN	-	EXPRESSION TAG	UNP P27487
A	780	SER	-	EXPRESSION TAG	UNP P27487
A	781	ALA	-	EXPRESSION TAG	UNP P27487
A	782	VAL	-	EXPRESSION TAG	UNP P27487
A	783	ASP	-	EXPRESSION TAG	UNP P27487
A	784	HIS	-	EXPRESSION TAG	UNP P27487
A	785	HIS	-	EXPRESSION TAG	UNP P27487
A	786	HIS	-	EXPRESSION TAG	UNP P27487
A	787	HIS	-	EXPRESSION TAG	UNP P27487
A	788	HIS	-	EXPRESSION TAG	UNP P27487
A	789	HIS	-	EXPRESSION TAG	UNP P27487

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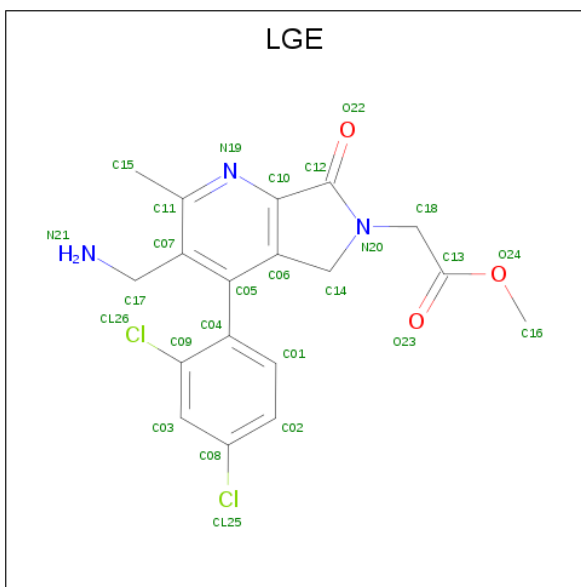
Chain	Residue	Modelled	Actual	Comment	Reference
B	37	GLU	-	EXPRESSION TAG	UNP P27487
B	38	PHE	-	EXPRESSION TAG	UNP P27487
B	767	PRO	-	EXPRESSION TAG	UNP P27487
B	768	LEU	-	EXPRESSION TAG	UNP P27487
B	769	GLU	-	EXPRESSION TAG	UNP P27487
B	770	GLN	-	EXPRESSION TAG	UNP P27487
B	771	LYS	-	EXPRESSION TAG	UNP P27487
B	772	LEU	-	EXPRESSION TAG	UNP P27487
B	773	ILE	-	EXPRESSION TAG	UNP P27487
B	774	SER	-	EXPRESSION TAG	UNP P27487
B	775	GLU	-	EXPRESSION TAG	UNP P27487
B	776	GLU	-	EXPRESSION TAG	UNP P27487
B	777	ASP	-	EXPRESSION TAG	UNP P27487
B	778	LEU	-	EXPRESSION TAG	UNP P27487
B	779	ASN	-	EXPRESSION TAG	UNP P27487
B	780	SER	-	EXPRESSION TAG	UNP P27487
B	781	ALA	-	EXPRESSION TAG	UNP P27487
B	782	VAL	-	EXPRESSION TAG	UNP P27487
B	783	ASP	-	EXPRESSION TAG	UNP P27487
B	784	HIS	-	EXPRESSION TAG	UNP P27487
B	785	HIS	-	EXPRESSION TAG	UNP P27487
B	786	HIS	-	EXPRESSION TAG	UNP P27487
B	787	HIS	-	EXPRESSION TAG	UNP P27487
B	788	HIS	-	EXPRESSION TAG	UNP P27487
B	789	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is methyl [3-(aminomethyl)-4-(2,4-dichlorophenyl)-2-methyl-7-oxo-5,7-dihydro-6H-pyrrolo[3,4-b]pyridin-6-yl]acetate (three-letter code: LGE) (formula: C<sub>18</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			26	18	2	3	3	
3	B	1	Total	C	Cl	N	O	
			26	18	2	3	3	

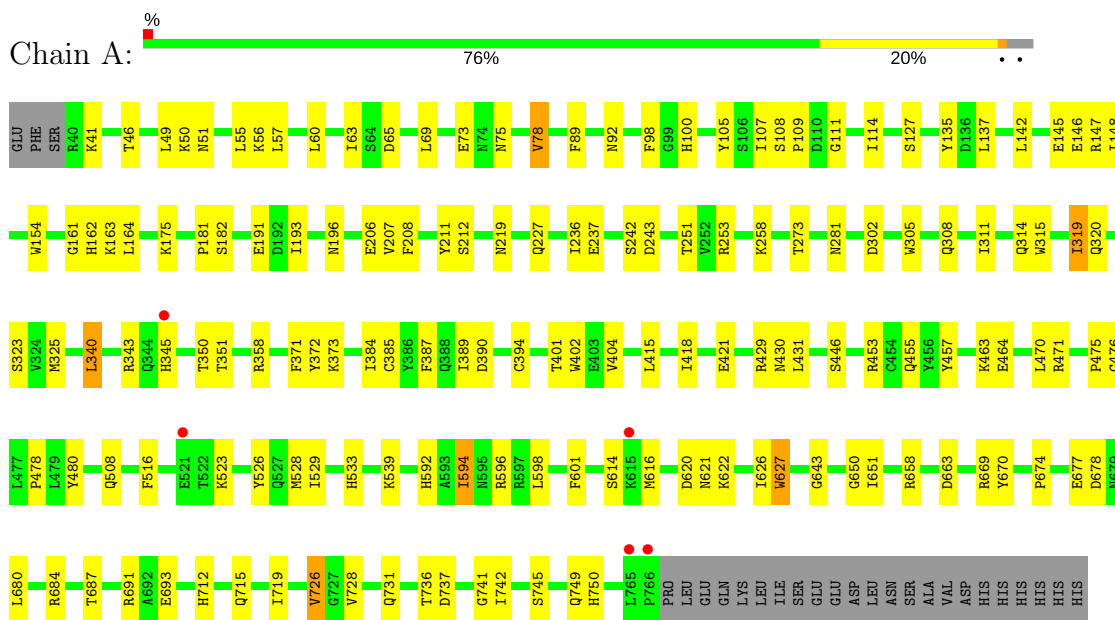
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O		
			208	208	0	0
4	B	223	Total	O		
			223	223	0	0

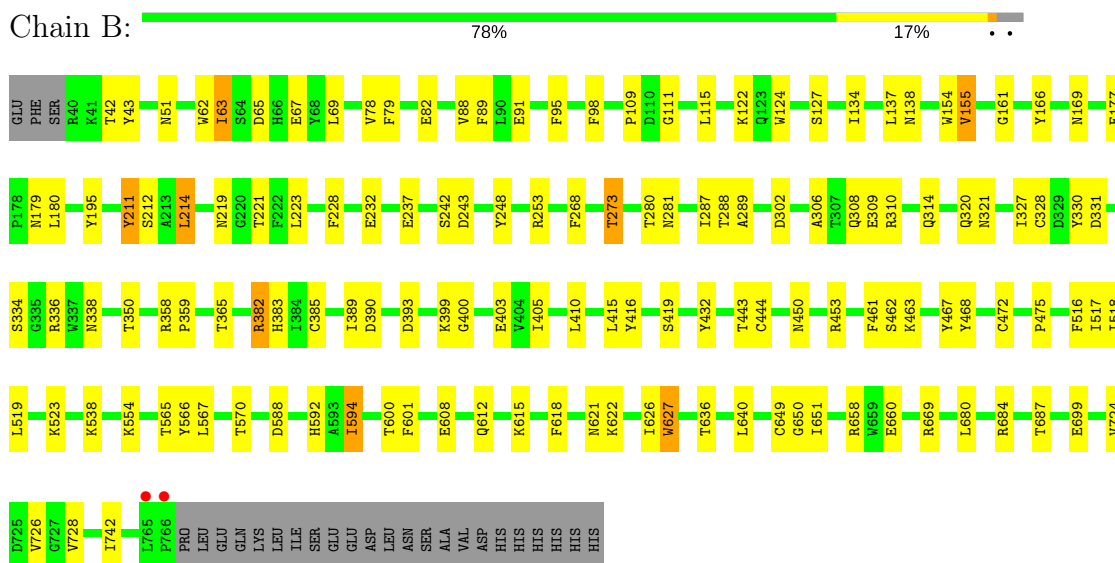
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Dipeptidyl peptidase 4



#### • Molecule 1: Dipeptidyl peptidase 4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.69Å 67.57Å 420.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 2.40 47.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (47.95-2.40) 96.1 (47.95-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 2.39Å)	Xtriage
Refinement program	PHENIX dev_606	Depositor
R, $R_{free}$	0.202 , 0.260 0.195 , 0.254	Depositor DCC
$R_{free}$ test set	2936 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.054 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.41	0/6068	0.56	0/8266
1	B	0.40	0/6064	0.56	0/8259
All	All	0.41	0/12132	0.56	0/16525

There are no bond length outliers.

There are no bond angle outliers.

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	5896	0	5536	112	0
1	B	5892	0	5514	89	0
2	A	98	0	90	5	0
2	B	98	0	90	2	0
3	A	26	0	17	0	0
3	B	26	0	17	0	0
4	A	208	0	0	4	0
4	B	223	0	0	2	0
All	All	12467	0	11264	199	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:HB2	1:B:308:GLN:OE1	1.66	0.95
1:A:319:ILE:HD12	1:A:319:ILE:H	1.32	0.94
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.52	0.90
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.56	0.85
1:A:135:TYR:HD1	1:A:142:LEU:HD12	1.42	0.83
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.65	0.79
1:A:191:GLU:O	1:A:193:ILE:HD12	1.83	0.77
1:A:281:ASN:HD21	2:A:2811:NAG:C2	2.00	0.75
1:B:177:GLU:HB2	1:B:180:LEU:HG	1.69	0.74
1:B:111:GLY:O	1:B:137:LEU:HD12	1.89	0.73
1:B:519:LEU:HB3	2:B:5201:NAG:H82	1.71	0.72
1:A:281:ASN:HD21	2:A:2811:NAG:C1	2.03	0.72
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.72	0.71
1:B:331:ASP:HB3	1:B:334:SER:HB3	1.76	0.68
1:B:155:VAL:HG13	1:B:166:TYR:HB3	1.76	0.67
1:B:327:ILE:HD13	1:B:389:ILE:HD12	1.76	0.66
1:B:517:ILE:HD12	1:B:612:GLN:HG3	1.76	0.66
1:A:281:ASN:ND2	2:A:2811:NAG:C1	2.60	0.65
1:B:658:ARG:HG3	1:B:687:THR:HG22	1.80	0.64
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.80	0.64
1:B:219:ASN:HB2	1:B:308:GLN:CD	2.18	0.63
1:B:63:ILE:HD13	1:B:69:LEU:HG	1.79	0.63
1:A:508:GLN:HE21	1:A:533:HIS:CE1	2.16	0.63
1:A:319:ILE:CD1	1:A:319:ILE:H	2.06	0.63
1:A:429:ARG:HD2	4:A:794:HOH:O	2.00	0.62
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.80	0.62
1:A:508:GLN:NE2	1:A:533:HIS:CE1	2.68	0.61
1:A:508:GLN:NE2	1:A:533:HIS:HE1	1.98	0.61
1:A:109:PRO:HD2	1:A:161:GLY:O	2.00	0.61
1:B:538:LYS:O	1:B:618:PHE:HA	2.00	0.61
1:A:78:VAL:HG12	1:A:89:PHE:HB2	1.81	0.61
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.01	0.60
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.83	0.59
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.02	0.58
1:A:56:LYS:O	1:A:57:LEU:HD23	2.04	0.58
1:B:518:ILE:O	1:B:519:LEU:HD12	2.03	0.58
1:A:471:ARG:HD2	1:A:480:TYR:HE2	1.69	0.57
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.38	0.57
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.34	0.57
1:B:122:LYS:HE2	1:B:124:TRP:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:OE1	1:A:92:ASN:ND2	2.38	0.57
1:A:107:ILE:HG22	1:A:108:SER:O	2.06	0.56
1:A:145:GLU:HG2	1:A:146:GLU:HG2	1.87	0.56
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.41	0.56
1:B:608:GLU:O	1:B:612:GLN:HG2	2.06	0.56
1:A:529:ILE:HD12	1:A:529:ILE:N	2.21	0.55
1:B:627:TRP:HA	1:B:651:ILE:O	2.07	0.55
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.89	0.55
1:A:60:LEU:HD12	1:A:60:LEU:O	2.06	0.55
1:A:314:GLN:HG2	1:A:325:MET:HG3	1.88	0.55
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.42	0.55
1:B:626:ILE:O	1:B:650:GLY:HA2	2.07	0.54
1:A:471:ARG:HD2	1:A:480:TYR:CE2	2.43	0.54
1:B:622:LYS:HB2	1:B:622:LYS:NZ	2.23	0.54
1:A:135:TYR:CD1	1:A:142:LEU:HD12	2.32	0.53
1:A:684:ARG:HH11	1:A:684:ARG:HG3	1.73	0.53
1:B:65:ASP:OD1	1:B:463:LYS:O	2.26	0.53
1:B:382:ARG:H	1:B:403:GLU:HG2	1.74	0.53
1:B:658:ARG:NH2	4:B:854:HOH:O	2.42	0.53
1:B:415:LEU:HD23	1:B:415:LEU:C	2.29	0.53
1:B:726:VAL:O	1:B:726:VAL:HG22	2.08	0.53
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.39	0.53
1:B:88:VAL:HG21	1:B:91:GLU:HG2	1.90	0.52
1:B:62:TRP:CE3	1:B:462:SER:HB3	2.44	0.52
1:B:115:LEU:HD23	1:B:134:ILE:HG12	1.91	0.52
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.45	0.51
1:A:243:ASP:HB3	4:A:816:HOH:O	2.09	0.51
1:A:163:LYS:NZ	1:A:273:THR:HG22	2.26	0.51
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.93	0.51
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.46	0.51
1:B:95:PHE:HB3	1:B:98:PHE:HB2	1.92	0.51
1:B:658:ARG:HG3	1:B:687:THR:CG2	2.41	0.50
1:A:715:GLN:O	1:A:719:ILE:HG13	2.10	0.50
1:A:46:THR:O	1:A:50:LYS:HB2	2.11	0.50
1:A:41:LYS:O	1:A:508:GLN:HB2	2.11	0.50
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.95	0.49
1:A:596:ARG:HA	1:A:670:TYR:O	2.12	0.49
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.30	0.49
1:B:519:LEU:HD23	2:B:5201:NAG:H82	1.93	0.49
1:B:636:THR:HG21	1:B:651:ILE:O	2.11	0.49
1:A:594:ILE:HG23	1:A:594:ILE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TRP:O	1:A:323:SER:HB2	2.12	0.49
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.12	0.49
1:A:147:ARG:HE	2:A:1501:NAG:H83	1.76	0.49
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.48	0.48
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.47	0.48
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.95	0.48
1:B:82:GLU:HB2	1:B:467:TYR:OH	2.14	0.48
1:A:643:GLY:HA2	4:A:936:HOH:O	2.13	0.48
1:A:73:GLU:O	1:A:73:GLU:HG2	2.13	0.48
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.97	0.48
1:A:242:SER:OG	1:A:243:ASP:N	2.47	0.47
1:B:195:TYR:HB2	1:B:228:PHE:HB2	1.96	0.47
1:B:383:HIS:CE1	1:B:399:LYS:HA	2.48	0.47
1:A:111:GLY:O	1:A:137:LEU:HD12	2.14	0.47
1:A:446:SER:HB2	1:A:457:TYR:CE2	2.49	0.47
1:B:288:THR:HG22	1:B:289:ALA:O	2.14	0.47
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.15	0.47
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.50	0.47
1:B:612:GLN:O	1:B:615:LYS:HB2	2.14	0.47
1:A:415:LEU:HD23	1:A:415:LEU:C	2.36	0.47
1:B:383:HIS:HE1	1:B:400:GLY:O	1.97	0.47
1:B:309:GLU:HB3	1:B:330:TYR:HB3	1.97	0.46
1:A:351:THR:OG1	1:A:592:HIS:CD2	2.69	0.46
1:A:457:TYR:CD1	1:A:470:LEU:HD22	2.50	0.46
1:A:684:ARG:NH1	1:A:684:ARG:HG3	2.31	0.46
1:B:221:THR:O	1:B:273:THR:HB	2.15	0.46
1:B:42:THR:HG23	1:B:570:THR:OG1	2.16	0.46
1:B:566:TYR:CE2	1:B:567:LEU:HD23	2.51	0.46
1:B:517:ILE:CD1	1:B:612:GLN:HG3	2.45	0.46
1:B:42:THR:CG2	1:B:570:THR:OG1	2.64	0.46
1:B:640:LEU:HA	1:B:640:LEU:HD23	1.80	0.46
1:B:640:LEU:HD11	1:B:650:GLY:CA	2.45	0.45
1:A:258:LYS:HD2	1:B:248:TYR:CZ	2.51	0.45
1:B:328:CYS:HA	1:B:338:ASN:O	2.16	0.45
1:A:526:TYR:HE1	1:A:528:MET:CE	2.30	0.45
1:A:741:GLY:O	1:A:742:ILE:C	2.55	0.45
1:B:389:ILE:O	1:B:390:ASP:HB2	2.17	0.45
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.97	0.45
1:A:674:PRO:C	1:A:680:LEU:HB2	2.37	0.45
1:A:693:GLU:OE2	1:A:726:VAL:HG22	2.16	0.45
1:A:516:PHE:CE1	1:A:523:LYS:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:OE2	1:A:253:ARG:HD3	2.17	0.45
1:A:401:THR:HG22	1:A:401:THR:O	2.16	0.45
1:A:463:LYS:O	1:A:464:GLU:HB2	2.17	0.45
1:A:453:ARG:HG3	1:A:476:GLY:HA3	1.98	0.45
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.99	0.45
1:A:691:ARG:NE	4:A:814:HOH:O	2.50	0.45
1:B:177:GLU:HB2	1:B:180:LEU:CG	2.44	0.44
1:A:236:ILE:HD12	1:A:237:GLU:H	1.81	0.44
1:A:340:LEU:HD23	1:A:343:ARG:NH1	2.32	0.44
1:B:109:PRO:HD2	1:B:161:GLY:O	2.17	0.44
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.98	0.44
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.52	0.44
1:B:453:ARG:O	1:B:475:PRO:HD2	2.18	0.44
1:B:594:ILE:HG23	1:B:594:ILE:O	2.17	0.44
1:B:327:ILE:CD1	1:B:389:ILE:HD12	2.44	0.44
1:A:539:LYS:HB3	1:A:620:ASP:HB2	1.99	0.44
1:A:107:ILE:HD11	1:A:114:ILE:HD12	2.00	0.44
1:A:358:ARG:HB3	1:A:358:ARG:NH1	2.33	0.43
1:A:60:LEU:C	1:A:60:LEU:HD12	2.39	0.43
1:B:43:TYR:CD2	1:B:565:THR:HG22	2.52	0.43
1:A:146:GLU:HG3	1:A:181:PRO:N	2.34	0.43
1:A:148:ILE:HD11	1:A:164:LEU:HD13	2.00	0.43
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.83	0.43
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.54	0.43
1:B:214:LEU:HG	1:B:223:LEU:HD11	2.00	0.43
1:A:526:TYR:HE1	1:A:528:MET:HE2	1.82	0.43
1:B:237:GLU:CG	1:B:253:ARG:HG2	2.40	0.43
1:B:600:THR:OG1	1:B:601:PHE:N	2.49	0.43
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.43
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.54	0.43
1:A:55:LEU:HD22	1:A:478:PRO:HG2	2.01	0.43
1:B:127:SER:HB3	1:B:211:TYR:CG	2.53	0.43
1:B:680:LEU:HD11	1:B:684:ARG:NE	2.34	0.43
1:A:325:MET:CE	1:A:371:PHE:CZ	3.02	0.43
1:A:281:ASN:HD21	2:A:2811:NAG:H2	1.81	0.43
1:A:387:PHE:CE2	1:A:394:CYS:HB3	2.54	0.42
1:A:389:ILE:O	1:A:390:ASP:HB2	2.18	0.42
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.02	0.42
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.54	0.42
1:B:179:ASN:ND2	1:B:179:ASN:H	2.16	0.42
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ILE:HD13	1:B:419:SER:HA	2.01	0.42
1:A:65:ASP:OD1	1:A:463:LYS:O	2.38	0.42
1:A:219:ASN:HB2	1:A:308:GLN:OE1	2.19	0.42
1:B:365:THR:HG22	1:B:410:LEU:HD21	2.02	0.42
1:B:405:ILE:HD12	1:B:405:ILE:N	2.35	0.42
1:A:626:ILE:O	1:A:650:GLY:HA2	2.20	0.42
1:A:745:SER:O	1:A:749:GLN:HG3	2.20	0.42
1:B:280:THR:HG22	1:B:281:ASN:O	2.19	0.42
1:B:358:ARG:O	1:B:359:PRO:C	2.58	0.41
1:A:693:GLU:HG2	1:A:726:VAL:HG21	2.01	0.41
1:B:67:GLU:HA	1:B:79:PHE:O	2.20	0.41
1:B:268:PHE:HD2	1:B:287:ILE:HB	1.85	0.41
1:B:415:LEU:HD23	1:B:416:TYR:N	2.36	0.41
1:A:614:SER:O	1:A:616:MET:O	2.38	0.41
1:B:169:ASN:N	1:B:169:ASN:HD22	2.18	0.41
1:B:621:ASN:N	1:B:621:ASN:OD1	2.52	0.41
1:A:627:TRP:HA	1:A:651:ILE:O	2.20	0.41
1:A:750:HIS:CG	1:B:724:VAL:HG22	2.55	0.41
1:B:516:PHE:CD1	1:B:523:LYS:HG2	2.55	0.41
1:B:588:ASP:O	1:B:592:HIS:HB2	2.21	0.41
1:A:63:ILE:HG21	1:A:69:LEU:HG	2.03	0.41
1:A:736:THR:O	1:A:737:ASP:HB2	2.21	0.41
1:A:594:ILE:HG23	1:A:598:LEU:HD23	2.03	0.41
1:A:163:LYS:NZ	1:A:273:THR:CG2	2.84	0.40
1:A:207:VAL:HG12	1:A:208:PHE:CD1	2.56	0.40
1:A:105:TYR:C	1:A:105:TYR:CD1	2.94	0.40
1:A:372:TYR:N	1:A:372:TYR:CD1	2.89	0.40
1:A:430:ASN:ND2	1:A:446:SER:OG	2.43	0.40
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.86	0.40
1:A:73:GLU:HB3	1:A:75:ASN:HD22	1.86	0.40
1:B:450:ASN:HB3	4:B:801:HOH:O	2.21	0.40
1:B:608:GLU:OE1	1:B:608:GLU:HA	2.21	0.40
1:B:242:SER:OG	1:B:243:ASP:N	2.52	0.40
1:A:251:THR:HG21	1:A:253:ARG:NH1	2.36	0.40
1:A:418:ILE:HD13	1:A:431:LEU:HA	2.03	0.40
1:A:726:VAL:HG13	1:A:728:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

## 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	725/753 (96%)	683 (94%)	42 (6%)	0	100	100
1	B	725/753 (96%)	691 (95%)	32 (4%)	2 (0%)	43	58
All	All	1450/1506 (96%)	1374 (95%)	74 (5%)	2 (0%)	53	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	138	ASN
1	B	742	ILE

### 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	631/677 (93%)	615 (98%)	16 (2%)	50	71
1	B	629/677 (93%)	610 (97%)	19 (3%)	44	65
All	All	1260/1354 (93%)	1225 (97%)	35 (3%)	47	67

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	78	VAL
1	A	162	HIS
1	A	319	ILE

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Mol	Chain	Res	Type
1	A	340	LEU
1	A	345	HIS
1	A	350	THR
1	A	373	LYS
1	A	385	CYS
1	A	594	ILE
1	A	621	ASN
1	A	622	LYS
1	A	627	TRP
1	A	677	GLU
1	A	726	VAL
1	A	731	GLN
1	B	51	ASN
1	B	63	ILE
1	B	155	VAL
1	B	211	TYR
1	B	214	LEU
1	B	232	GLU
1	B	273	THR
1	B	321	ASN
1	B	336	ARG
1	B	350	THR
1	B	382	ARG
1	B	385	CYS
1	B	393	ASP
1	B	443	THR
1	B	472	CYS
1	B	554	LYS
1	B	594	ILE
1	B	627	TRP
1	B	660	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	123	GLN
1	A	247	GLN
1	A	281	ASN
1	A	314	GLN
1	A	430	ASN
1	A	508	GLN

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Mol	Chain	Res	Type
1	A	533	HIS
1	A	586	GLN
1	A	592	HIS
1	A	731	GLN
1	B	169	ASN
1	B	179	ASN
1	B	383	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 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	LGE	A	1	-	27,28,28	1.25	4 (14%)	35,41,41	1.39	6 (17%)
2	NAG	A	1501	1	14,14,15	0.52	0	17,19,21	0.83	1 (5%)
2	NAG	A	2191	1	14,14,15	0.62	0	17,19,21	1.08	1 (5%)
2	NAG	A	2291	1,2	14,14,15	0.54	0	17,19,21	0.77	0
2	NAG	A	2292	2	14,14,15	0.62	0	17,19,21	1.05	1 (5%)
2	NAG	A	2811	-	14,14,15	0.61	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	5201	1	14,14,15	0.46	0	17,19,21	0.85	1 (5%)
2	NAG	A	851	1	14,14,15	0.57	0	17,19,21	1.12	1 (5%)
2	NAG	B	1501	1	14,14,15	0.62	0	17,19,21	1.79	3 (17%)
3	LGE	B	2	-	27,28,28	1.05	1 (3%)	35,41,41	1.44	6 (17%)
2	NAG	B	2191	1	14,14,15	0.53	0	17,19,21	0.82	0
2	NAG	B	2291	1,2	14,14,15	0.55	0	17,19,21	1.09	2 (11%)
2	NAG	B	2292	2	14,14,15	0.50	0	17,19,21	1.64	1 (5%)
2	NAG	B	5201	1	14,14,15	0.53	0	17,19,21	0.75	0
2	NAG	B	851	1	14,14,15	0.62	0	17,19,21	1.04	1 (5%)
2	NAG	B	921	1	14,14,15	0.45	0	17,19,21	1.52	3 (17%)

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	LGE	A	1	-	-	0/11/24/24	0/3/3/3
2	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2291	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2292	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2811	-	-	0/6/23/26	0/1/1/1
2	NAG	A	5201	1	-	0/6/23/26	0/1/1/1
2	NAG	A	851	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1501	1	1/1/5/7	0/6/23/26	0/1/1/1
3	LGE	B	2	-	-	0/11/24/24	0/3/3/3
2	NAG	B	2191	1	-	0/6/23/26	0/1/1/1
2	NAG	B	2291	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2292	2	-	0/6/23/26	0/1/1/1
2	NAG	B	5201	1	-	0/6/23/26	0/1/1/1
2	NAG	B	851	1	-	0/6/23/26	0/1/1/1
2	NAG	B	921	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	LGE	C04-C05	-2.40	1.47	1.50
3	A	1	LGE	C08-CL25	-2.03	1.70	1.74
3	A	1	LGE	C12-N20	2.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	LGE	C11-N19	2.78	1.38	1.34
3	B	2	LGE	C12-N20	3.28	1.41	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	NAG	O5-C1-C2	-4.96	104.67	111.52
3	B	2	LGE	C05-C06-C10	-3.48	118.55	120.11
2	B	2291	NAG	O5-C1-C2	-2.79	107.66	111.52
3	B	2	LGE	C15-C11-N19	-2.41	112.80	116.45
3	A	1	LGE	C10-N19-C11	-2.39	113.52	117.59
2	B	921	NAG	C4-C3-C2	-2.38	107.54	111.02
2	A	2811	NAG	O5-C1-C2	-2.30	108.34	111.52
3	A	1	LGE	C05-C06-C10	-2.25	119.10	120.11
3	A	1	LGE	C15-C11-N19	-2.20	113.12	116.45
3	B	2	LGE	C09-C03-C08	-2.14	116.40	118.72
3	B	2	LGE	C10-N19-C11	-2.04	114.12	117.59
2	B	2291	NAG	C2-N2-C7	-2.02	119.99	122.94
3	A	1	LGE	O24-C13-C18	2.11	113.95	110.25
3	A	1	LGE	C05-C07-C11	2.12	119.07	117.80
2	A	1501	NAG	O5-C5-C6	2.16	110.57	107.15
2	A	851	NAG	C1-O5-C5	2.16	115.16	112.19
2	A	2292	NAG	C1-O5-C5	2.17	115.18	112.19
3	B	2	LGE	C04-C05-C07	2.23	123.75	120.79
3	A	1	LGE	C04-C05-C07	2.23	123.75	120.79
3	B	2	LGE	O24-C13-C18	2.30	114.28	110.25
2	B	921	NAG	O5-C5-C6	2.31	110.81	107.15
2	A	5201	NAG	C1-O5-C5	2.45	115.56	112.19
2	B	1501	NAG	C3-C4-C5	2.78	115.22	110.24
2	B	851	NAG	C1-O5-C5	3.04	116.38	112.19
2	A	2191	NAG	C1-O5-C5	3.18	116.56	112.19
2	B	1501	NAG	C4-C3-C2	3.74	116.49	111.02
2	B	921	NAG	C1-O5-C5	4.39	118.23	112.19
2	B	2292	NAG	C1-O5-C5	5.76	120.11	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1501	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	NAG	1	0
2	A	2811	NAG	4	0
2	B	5201	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	727/753 (96%)	-0.40	5 (0%)	87 86	28, 41, 64, 84	0
1	B	727/753 (96%)	-0.39	2 (0%)	93 93	29, 42, 64, 86	0
All	All	1454/1506 (96%)	-0.39	7 (0%)	90 89	28, 42, 64, 86	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	LEU	4.7
1	B	765	LEU	3.3
1	A	766	PRO	3.1
1	B	766	PRO	3.1
1	A	521	GLU	2.2
1	A	615	LYS	2.2
1	A	345	HIS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	2191	14/15	0.75	0.27	62,72,76,78	0
2	NAG	B	5201	14/15	0.80	0.26	50,72,75,77	0
2	NAG	B	2191	14/15	0.80	0.26	65,73,81,81	0
2	NAG	A	2292	14/15	0.85	0.23	56,69,83,83	0
2	NAG	B	1501	14/15	0.85	0.23	64,77,89,94	0
2	NAG	B	2292	14/15	0.87	0.28	55,77,84,88	0
2	NAG	B	921	14/15	0.89	0.21	68,71,75,75	0
2	NAG	A	1501	14/15	0.90	0.25	61,70,77,78	0
2	NAG	B	2291	14/15	0.90	0.12	40,55,61,67	0
2	NAG	A	5201	14/15	0.91	0.29	58,67,75,77	0
2	NAG	A	2811	14/15	0.92	0.25	64,70,74,75	0
2	NAG	A	851	14/15	0.95	0.12	40,43,47,48	0
3	LGE	B	2	26/26	0.95	0.19	31,40,52,53	0
2	NAG	A	2291	14/15	0.95	0.13	35,51,59,61	0
3	LGE	A	1	26/26	0.96	0.17	35,39,47,50	0
2	NAG	B	851	14/15	0.96	0.10	41,43,44,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.