



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:46 am GMT

PDB ID : 1HJX  
Title : Ligand-induced signalling and conformational change of the 39 kD glycoprotein from human articular chondrocytes  
Authors : Houston, D.R.; Recklies, A.D.; Krupa, J.C.; Van Aalten, D.M.F.  
Deposited on : 2003-02-28  
Resolution : 1.85 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

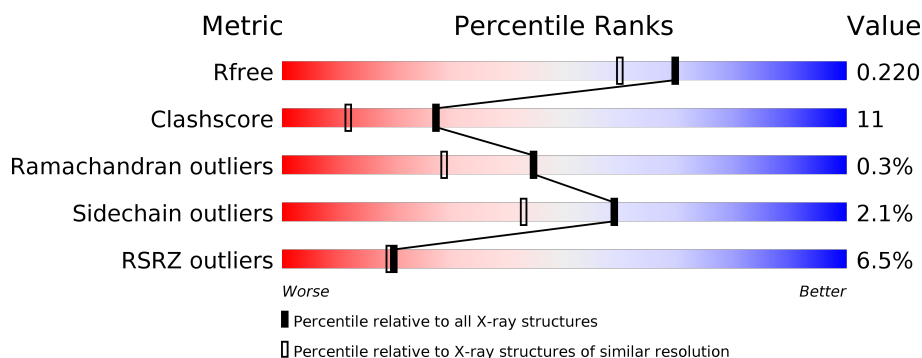
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	362	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	362	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	362	<div> <div>7%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	D	362	<div> <div>12%</div> <div>77%</div> <div>22%</div> <div>..</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	1385	-	-	-	X
4	GOL	A	1387	-	-	-	X
4	GOL	A	1388	-	-	X	X
4	GOL	A	1389	-	-	-	X
4	GOL	A	1390	-	-	X	X
4	GOL	A	1391	-	-	X	X
4	GOL	B	1389	-	-	X	X
4	GOL	B	1390	-	-	X	-
4	GOL	C	1388	-	-	-	X
4	GOL	C	1389	-	-	X	X
4	GOL	C	1390	-	-	X	X
4	GOL	C	1392	-	-	X	X
4	GOL	D	1385	-	-	-	X
4	GOL	D	1387	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13127 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 CHITINASE-3 LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	20	8	1
			2887	1842	498	536	11			
1	B	362	Total	C	N	O	S	10	6	1
			2884	1843	499	531	11			
1	C	359	Total	C	N	O	S	14	2	1
			2845	1817	492	525	11			
1	D	360	Total	C	N	O	S	31	6	1
			2870	1833	497	529	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	VARIANT	UNP P36222
B	311	ILE	THR	VARIANT	UNP P36222
C	311	ILE	THR	VARIANT	UNP P36222
D	311	ILE	THR	VARIANT	UNP P36222

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

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

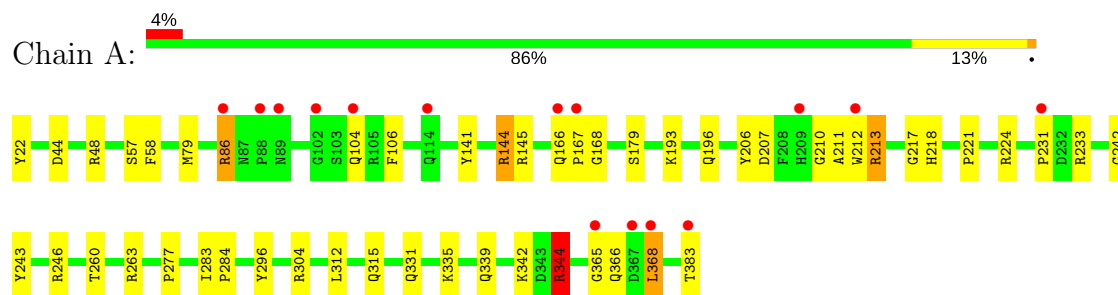
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	417	Total	O	0	0
			417	417		
5	B	448	Total	O	0	0
			448	448		
5	C	299	Total	O	0	0
			299	299		
5	D	229	Total	O	0	0
			229	229		

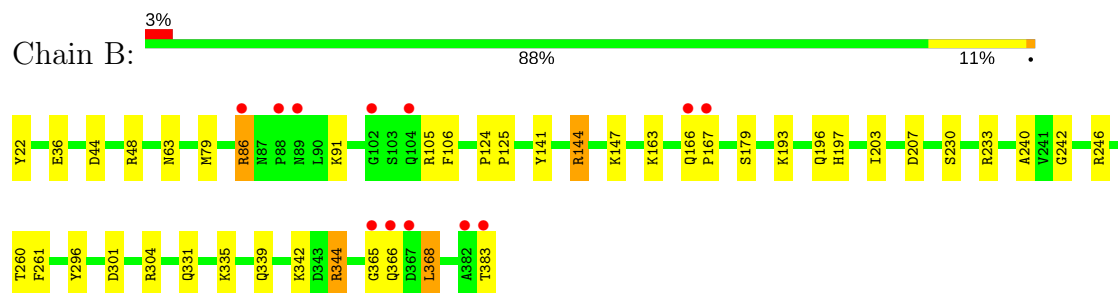
### 3 Residue-property plots [i](#)

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.

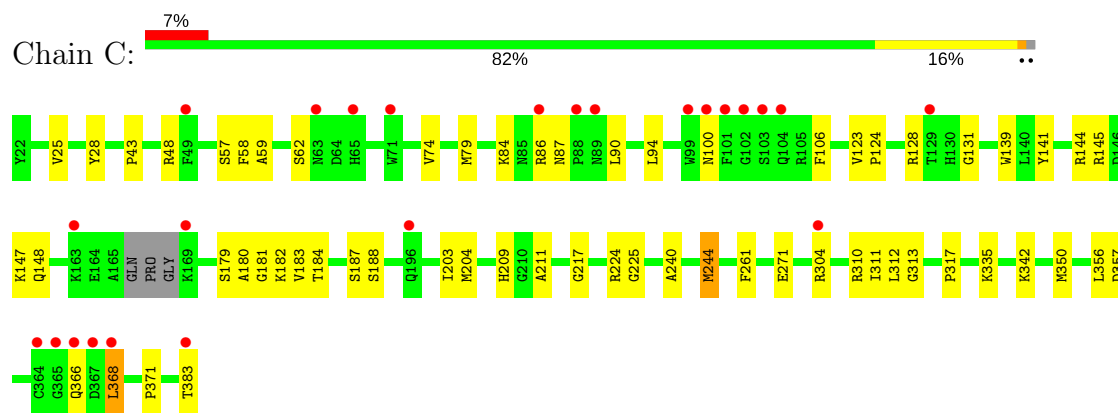
#### • Molecule 1: CHITINASE-3 LIKE PROTEIN 1



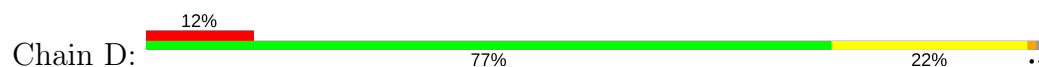
#### • Molecule 1: CHITINASE-3 LIKE PROTEIN 1



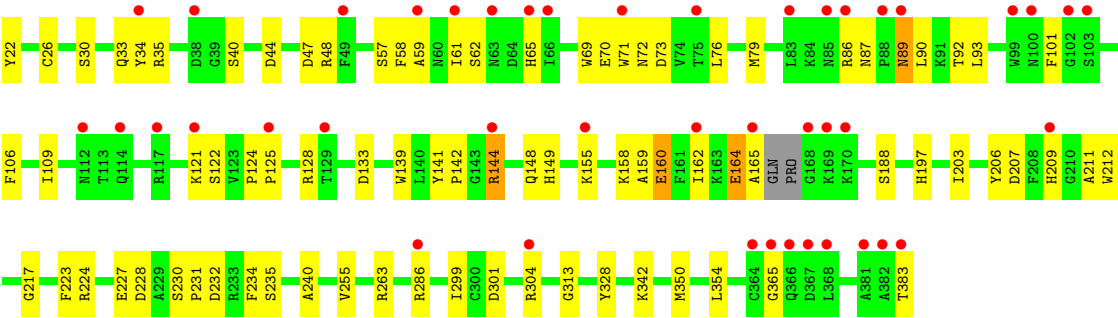
#### • Molecule 1: CHITINASE-3 LIKE PROTEIN 1



#### • Molecule 1: CHITINASE-3 LIKE PROTEIN 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.56Å 122.05Å 136.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 1.85 15.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (14.98-1.85) 99.0 (15.00-1.85)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 1.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.197 , 0.225 0.193 , 0.220	Depositor DCC
$R_{free}$ test set	728 reflections (0.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 68.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, SO4

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	0.65	0/2998	0.79	3/4061 (0.1%)
1	B	0.67	0/2984	0.78	1/4041 (0.0%)
1	C	0.55	0/2927	0.74	3/3963 (0.1%)
1	D	0.53	0/2969	0.69	0/4018
All	All	0.61	0/11878	0.75	7/16083 (0.0%)

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	C	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	344	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	C	310	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	168	GLY	N-CA-C	5.21	126.12	113.10
1	A	312	LEU	C-N-CA	-5.20	111.39	122.30
1	C	188	SER	N-CA-C	5.05	124.62	111.00
1	C	310	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	28	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2887	0	2798	61	0
1	B	2884	0	2807	48	0
1	C	2845	0	2764	69	0
1	D	2870	0	2785	70	0
2	A	28	0	25	0	0
2	B	28	0	25	4	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	5	0	0	0	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
4	A	36	0	48	24	0
4	B	12	0	16	11	0
4	C	30	0	40	39	0
4	D	18	0	24	9	0
5	A	417	0	0	21	0
5	B	448	0	0	14	0
5	C	299	0	0	10	0
5	D	229	0	0	8	0
All	All	13127	0	11382	262	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 11.

All (262) 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)
5:B:2409:HOH:O	4:C:1389:GOL:H31	1.50	1.09
1:C:48:ARG:HD2	1:C:86:ARG:HB3	1.47	0.93
1:A:315:GLN:NE2	1:D:313:GLY:H	1.66	0.93
1:A:315:GLN:HE21	1:D:313:GLY:H	0.96	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:H	4:C:1390:GOL:C1	1.85	0.89
1:A:166[A]:GLN:HG2	1:A:167:PRO:HD3	1.55	0.88
1:D:211:ALA:HB3	4:D:1387:GOL:H32	1.55	0.85
1:C:48:ARG:CD	1:C:86:ARG:HB3	2.07	0.84
1:B:44:ASP:H	1:B:79:MET:HE2	1.42	0.84
1:D:211:ALA:CB	4:D:1387:GOL:H32	2.08	0.83
4:A:1388:GOL:O3	1:D:228:ASP:HB3	1.77	0.82
1:C:147:LYS:HB3	4:C:1392:GOL:H2	1.60	0.82
1:D:148[A]:GLN:HG2	5:D:2064:HOH:O	1.81	0.81
1:A:210:GLY:O	1:A:231:PRO:HD2	1.81	0.81
1:C:148:GLN:HG2	4:C:1392:GOL:H11	1.61	0.80
1:A:315:GLN:HE21	1:D:313:GLY:N	1.78	0.80
1:A:366:GLN:HB3	1:A:368:LEU:HD23	1.62	0.80
1:C:148:GLN:HG2	4:C:1392:GOL:C1	2.10	0.80
1:A:213:ARG:HH11	1:A:213:ARG:HG3	1.47	0.80
1:D:159:ALA:HA	1:D:162:ILE:HD12	1.63	0.79
1:C:183:VAL:H	4:C:1390:GOL:H11	1.47	0.79
1:A:210:GLY:O	1:A:231:PRO:CD	2.32	0.78
1:A:231:PRO:HD2	5:A:2264:HOH:O	1.84	0.77
1:C:183:VAL:H	4:C:1390:GOL:H12	1.53	0.74
1:B:63:ASN:H	4:B:1390:GOL:H11	1.53	0.73
1:D:211:ALA:HB3	4:D:1387:GOL:C3	2.18	0.73
1:A:193:LYS:O	1:A:196[A]:GLN:HG2	1.89	0.73
1:A:335[A]:LYS:HE3	5:A:2186:HOH:O	1.89	0.72
1:A:335[B]:LYS:HE3	5:A:2368:HOH:O	1.89	0.72
1:A:246:ARG:NE	4:A:1388:GOL:O1	2.19	0.72
1:C:313:GLY:N	4:C:1389:GOL:O2	2.22	0.71
1:C:271:GLU:HG3	5:C:2195:HOH:O	1.89	0.71
1:D:212:TRP:CE3	1:D:231:PRO:HG3	2.26	0.71
1:C:183:VAL:HB	4:C:1390:GOL:H11	1.72	0.71
1:D:207[B]:ASP:OD2	1:D:263:ARG:NH2	2.24	0.71
4:C:1389:GOL:H11	5:C:2078:HOH:O	1.92	0.70
1:B:166:GLN:HB2	1:B:167:PRO:HD3	1.74	0.70
1:B:207:ASP:OD2	4:B:1389:GOL:H12	1.91	0.69
1:B:335[A]:LYS:HE2	5:B:2426:HOH:O	1.92	0.69
2:B:1383:NAG:O6	4:B:1390:GOL:H12	1.93	0.69
1:A:331[B]:GLN:OE1	5:A:2363:HOH:O	2.10	0.69
1:C:209:HIS:NE2	4:C:1391:GOL:H11	2.09	0.68
1:D:61:ILE:HG21	1:D:109:ILE:HD13	1.76	0.68
1:A:233:ARG:NH2	4:A:1390:GOL:H31	2.09	0.67
1:C:183:VAL:CB	4:C:1390:GOL:H11	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LYS:HD2	5:C:2259:HOH:O	1.95	0.67
1:B:163:LYS:HA	1:B:166:GLN:HG3	1.77	0.67
1:C:148:GLN:HG2	4:C:1392:GOL:O1	1.96	0.66
1:B:44:ASP:H	1:B:79:MET:CE	2.09	0.66
1:D:89:ASN:HD22	1:D:89:ASN:N	1.92	0.66
1:B:144:ARG:NH1	5:B:2201:HOH:O	2.29	0.65
1:C:144:ARG:HG2	1:C:187:SER:HB2	1.77	0.65
1:D:142:PRO:HB2	1:D:188:SER:HB2	1.79	0.64
1:B:331:GLN:O	1:B:335[A]:LYS:HG3	1.97	0.64
1:D:30:SER:O	1:D:33:GLN:HG2	1.98	0.64
1:A:104:GLN:HB2	5:A:2129:HOH:O	1.96	0.63
1:C:312:LEU:HB2	4:C:1389:GOL:H2	1.80	0.63
1:D:148[A]:GLN:HG3	1:D:149:HIS:N	2.11	0.63
1:D:203:ILE:HD11	1:D:240:ALA:HB1	1.79	0.63
1:B:44:ASP:HB3	1:B:79:MET:HE3	1.80	0.63
1:A:366:GLN:HB3	1:A:368:LEU:CD2	2.29	0.62
4:A:1391:GOL:H12	5:A:2416:HOH:O	1.98	0.62
1:A:166[A]:GLN:CG	1:A:167:PRO:HD3	2.26	0.62
1:B:144:ARG:HH21	1:B:144:ARG:HG3	1.65	0.62
1:C:144:ARG:CG	1:C:187:SER:HB2	2.30	0.62
1:A:315:GLN:NE2	5:A:2349:HOH:O	2.32	0.62
1:B:44:ASP:N	1:B:79:MET:HE2	2.13	0.61
1:D:158:LYS:O	1:D:162:ILE:HG13	2.02	0.60
1:D:206:TYR:O	4:D:1385:GOL:H11	2.02	0.59
1:C:366:GLN:HB3	1:C:368:LEU:HD23	1.84	0.59
1:A:243:TYR:HD1	4:A:1388:GOL:H12	1.67	0.59
1:C:366:GLN:HB3	1:C:368:LEU:CD2	2.32	0.58
1:C:87:ASN:ND2	1:C:90:LEU:HB2	2.19	0.58
1:C:311:ILE:HG23	4:C:1389:GOL:H12	1.84	0.58
1:D:148[B]:GLN:NE2	5:D:2067:HOH:O	2.35	0.58
4:A:1391:GOL:C1	5:A:2416:HOH:O	2.50	0.58
1:C:312:LEU:HB2	4:C:1389:GOL:C2	2.34	0.58
1:A:213:ARG:NH1	1:A:213:ARG:HG3	2.18	0.58
1:D:92:THR:C	1:D:93:LEU:HD12	2.24	0.58
1:A:221:PRO:HG3	4:A:1391:GOL:H2	1.86	0.58
1:C:100:ASN:ND2	5:C:2054:HOH:O	2.36	0.57
1:D:69:TRP:HB3	5:D:2005:HOH:O	2.04	0.57
1:A:242:GLY:C	4:A:1388:GOL:H31	2.25	0.57
1:B:63:ASN:H	4:B:1390:GOL:C1	2.18	0.57
1:D:158:LYS:HG3	1:D:162:ILE:HD11	1.87	0.56
1:D:155:LYS:HG3	1:D:197:HIS:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ALA:H	4:C:1388:GOL:C1	2.18	0.56
1:B:261:PHE:CZ	4:B:1389:GOL:H2	2.41	0.56
1:A:44:ASP:CG	1:A:79:MET:HE1	2.27	0.56
1:C:141:TYR:CE1	1:C:179:SER:HB2	2.40	0.56
1:A:44:ASP:H	1:A:79:MET:HE2	1.71	0.55
1:B:44:ASP:CG	1:B:79:MET:HE1	2.27	0.55
1:D:235:SER:O	4:D:1386:GOL:H11	2.06	0.55
1:A:144:ARG:NH1	5:A:2177:HOH:O	2.39	0.55
1:C:144:ARG:O	4:C:1392:GOL:C3	2.54	0.55
1:C:183:VAL:N	4:C:1390:GOL:H11	2.20	0.55
1:D:209:HIS:HA	4:D:1387:GOL:O3	2.07	0.55
1:C:211:ALA:HB2	1:C:217:GLY:HA3	1.88	0.54
1:C:182:LYS:N	4:C:1390:GOL:H12	2.23	0.54
1:B:36:GLU:HG3	5:B:2031:HOH:O	2.08	0.54
1:D:89:ASN:ND2	1:D:89:ASN:N	2.56	0.54
1:A:243:TYR:HA	4:A:1388:GOL:H12	1.88	0.54
1:B:260:THR:O	1:B:296:TYR:HB2	2.07	0.54
1:B:342:LYS:NZ	1:B:383:THR:N	2.55	0.54
1:B:144:ARG:HH21	1:B:144:ARG:CG	2.21	0.53
1:B:335[B]:LYS:HD2	5:B:2404:HOH:O	2.08	0.53
1:A:233:ARG:CZ	4:A:1390:GOL:C3	2.86	0.53
1:D:87:ASN:ND2	1:D:90:LEU:HB2	2.23	0.53
1:C:204:MET:HE3	5:C:2133:HOH:O	2.08	0.53
1:D:211:ALA:HB2	1:D:217:GLY:HA3	1.91	0.52
1:A:144:ARG:HG2	1:A:144:ARG:NH1	2.23	0.52
4:A:1387:GOL:H32	5:A:2411:HOH:O	2.08	0.52
1:A:246:ARG:HH21	4:A:1388:GOL:H32	1.74	0.52
1:D:70:GLU:N	1:D:73:ASP:OD2	2.39	0.52
1:B:207:ASP:CG	4:B:1389:GOL:H12	2.30	0.52
1:D:141:TYR:OH	4:D:1385:GOL:H32	2.10	0.52
1:C:144:ARG:O	4:C:1392:GOL:H32	2.10	0.52
1:C:148:GLN:HE21	4:C:1392:GOL:H11	1.75	0.52
1:D:133:ASP:HB3	5:D:2056:HOH:O	2.09	0.52
1:D:122:SER:O	1:D:125:PRO:HG2	2.10	0.52
1:C:144:ARG:NH1	5:C:2097:HOH:O	2.43	0.51
1:D:71:TRP:CZ3	1:D:72:ASN:HB3	2.46	0.51
1:B:366:GLN:HB3	1:B:368:LEU:HD23	1.93	0.51
1:C:147:LYS:HB3	4:C:1392:GOL:C2	2.38	0.51
1:A:206:TYR:O	4:A:1386:GOL:H32	2.11	0.51
1:B:86:ARG:HH11	1:B:86:ARG:HG2	1.74	0.51
4:D:1386:GOL:O1	5:D:2228:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:CD	1:A:86:ARG:HB3	2.40	0.51
1:C:183:VAL:N	4:C:1390:GOL:C1	2.67	0.51
1:D:342:LYS:NZ	1:D:383:THR:N	2.59	0.50
2:B:1383:NAG:C6	4:B:1390:GOL:H12	2.41	0.50
1:D:149:HIS:HD2	5:D:2068:HOH:O	1.95	0.50
1:C:124:PRO:O	1:C:128:ARG:HG2	2.12	0.50
1:A:233:ARG:CZ	4:A:1390:GOL:H31	2.42	0.50
1:C:312:LEU:HB2	4:C:1389:GOL:C3	2.42	0.50
1:C:311:ILE:CG2	4:C:1389:GOL:H12	2.42	0.50
1:D:48:ARG:CD	1:D:86:ARG:HB3	2.42	0.50
1:D:255:VAL:HG12	1:D:350:MET:HB2	1.94	0.49
1:B:301[A]:ASP:OD1	1:B:304:ARG:NH1	2.45	0.49
1:B:193:LYS:HA	1:B:196:GLN:HE21	1.76	0.49
1:C:312:LEU:N	4:C:1389:GOL:H2	2.28	0.48
1:B:48:ARG:NH1	5:B:2058:HOH:O	2.44	0.48
1:B:44:ASP:CG	1:B:79:MET:CE	2.82	0.48
1:B:230:SER:HA	5:B:2301:HOH:O	2.13	0.48
1:C:357:ASP:OD1	1:C:371:PRO:HD2	2.13	0.48
1:B:342:LYS:HZ1	1:B:383:THR:N	2.10	0.48
1:C:312:LEU:HB2	4:C:1389:GOL:H32	1.94	0.48
1:C:203:ILE:HD11	1:C:240:ALA:HB1	1.95	0.47
1:B:48:ARG:NE	5:B:2057:HOH:O	2.47	0.47
1:C:183:VAL:CG2	4:C:1390:GOL:H11	2.44	0.47
1:D:35:ARG:O	1:D:40:SER:HB2	2.14	0.47
4:A:1389:GOL:H11	5:A:2414:HOH:O	2.13	0.47
1:C:184:THR:H	4:C:1390:GOL:C3	2.27	0.47
1:D:86:ARG:HG2	1:D:86:ARG:HH11	1.79	0.47
1:A:144:ARG:HG3	5:A:2176:HOH:O	2.14	0.47
1:D:124:PRO:O	1:D:128:ARG:HG2	2.15	0.47
1:D:33:GLN:HG3	1:D:34:TYR:N	2.30	0.47
1:A:207:ASP:HB3	5:A:2282:HOH:O	2.15	0.47
1:D:211:ALA:H	4:D:1387:GOL:H32	1.80	0.46
2:B:1383:NAG:H62	4:B:1390:GOL:H32	1.97	0.46
1:A:260:THR:O	1:A:296:TYR:HB2	2.15	0.46
1:B:44:ASP:CB	1:B:79:MET:HE3	2.45	0.46
1:A:166[A]:GLN:CG	1:A:167:PRO:CD	2.93	0.46
1:A:44:ASP:N	1:A:79:MET:HE2	2.30	0.46
1:D:224:ARG:HG2	1:D:224:ARG:O	2.15	0.46
1:B:233:ARG:HB2	5:B:2288:HOH:O	2.15	0.46
1:A:144:ARG:HH11	1:A:144:ARG:HG2	1.80	0.46
1:C:180:ALA:H	4:C:1388:GOL:H12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1389:GOL:C1	5:C:2291:HOH:O	2.64	0.46
1:C:183:VAL:N	4:C:1390:GOL:H12	2.26	0.46
2:B:1384:NAG:HN2	4:B:1390:GOL:H32	1.80	0.46
1:D:223:PHE:HB2	1:D:313:GLY:O	2.16	0.46
1:D:62:SER:O	1:D:65[A]:HIS:ND1	2.49	0.46
1:B:366:GLN:HB3	1:B:368:LEU:CD2	2.45	0.45
1:B:86:ARG:HG2	1:B:86:ARG:NH1	2.31	0.45
1:D:232:ASP:OD1	1:D:234:PHE:N	2.49	0.45
1:A:342:LYS:NZ	1:A:383:THR:N	2.63	0.45
1:B:22:TYR:CZ	1:B:342:LYS:HG2	2.51	0.45
1:D:124:PRO:N	1:D:125:PRO:HD2	2.31	0.45
4:A:1388:GOL:H11	5:A:2412:HOH:O	2.15	0.45
1:D:144:ARG:HG2	5:D:2063:HOH:O	2.15	0.45
4:A:1388:GOL:C1	5:A:2412:HOH:O	2.64	0.45
1:C:342:LYS:NZ	1:C:383:THR:N	2.65	0.45
1:A:243:TYR:HD1	4:A:1388:GOL:C1	2.29	0.45
1:C:183:VAL:HG23	4:C:1390:GOL:H11	1.99	0.45
1:A:233:ARG:CZ	4:A:1390:GOL:H32	2.47	0.45
1:B:203:ILE:HD11	1:B:240:ALA:HB1	1.99	0.45
1:C:74:VAL:HG23	5:C:2037:HOH:O	2.17	0.45
1:C:368:LEU:HA	5:C:2278:HOH:O	2.17	0.45
1:A:211:ALA:HB2	1:A:217:GLY:HA3	1.99	0.44
1:D:164:GLU:O	1:D:165:ALA:HB2	2.18	0.44
1:B:207:ASP:OD2	4:B:1389:GOL:H31	2.17	0.44
1:D:57:SER:HA	1:D:58:PHE:HA	1.71	0.44
1:A:207:ASP:OD1	1:A:263:ARG:NH1	2.50	0.44
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.82	0.44
1:D:69:TRP:N	1:D:73:ASP:OD2	2.40	0.44
1:C:43:PRO:HB2	1:C:79:MET:HB2	2.00	0.44
1:D:26:CYS:HB3	1:D:354:LEU:HG	1.99	0.44
4:C:1389:GOL:H2	5:C:2246:HOH:O	2.17	0.44
1:D:71:TRP:CE3	1:D:72:ASN:HB3	2.53	0.44
1:A:213:ARG:C	1:A:213:ARG:HD2	2.38	0.44
1:A:344:ARG:HD2	5:A:2375:HOH:O	2.16	0.44
1:B:335[A]:LYS:HD2	5:B:2405:HOH:O	2.17	0.44
1:D:301:ASP:HA	1:D:304[A]:ARG:NH1	2.33	0.44
1:A:141:TYR:CE1	1:A:179:SER:HB2	2.54	0.43
1:D:61:ILE:CG2	1:D:109:ILE:HD13	2.46	0.43
1:A:277:PRO:HB3	1:C:144:ARG:HD3	1.99	0.43
4:A:1388:GOL:O3	1:D:227[A]:GLU:OE2	2.17	0.43
1:D:232:ASP:OD1	1:D:232:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ASP:HA	1:D:304[B]:ARG:NH1	2.33	0.43
1:B:261:PHE:CE2	4:B:1389:GOL:H2	2.54	0.43
1:C:139:TRP:O	1:C:141:TYR:HA	2.19	0.43
4:A:1388:GOL:O2	1:D:227[A]:GLU:OE2	2.35	0.43
1:C:184:THR:H	4:C:1390:GOL:H31	1.83	0.43
1:D:299:ILE:HD13	1:D:328:TYR:CB	2.49	0.43
1:A:144:ARG:HH11	1:A:144:ARG:CG	2.30	0.42
1:B:242:GLY:O	1:B:246[B]:ARG:HG3	2.19	0.42
1:C:203:ILE:HD12	1:C:244:MET:HG3	2.00	0.42
1:C:209:HIS:CE1	4:C:1391:GOL:H11	2.54	0.42
1:A:212:TRP:CZ2	1:A:231:PRO:HA	2.54	0.42
1:C:123:VAL:HB	1:C:124:PRO:HD3	2.01	0.42
1:A:57:SER:HA	1:A:58:PHE:HA	1.69	0.42
1:C:57:SER:HB3	1:C:58:PHE:CD1	2.54	0.42
1:D:342:LYS:HZ2	1:D:383:THR:N	2.17	0.42
1:A:144:ARG:NH2	5:A:2173:HOH:O	2.52	0.42
1:C:144:ARG:HG3	1:C:187:SER:HB2	2.02	0.42
1:D:121:LYS:HA	1:D:160:GLU:OE1	2.20	0.42
1:B:144:ARG:NH2	1:B:144:ARG:CG	2.81	0.42
1:C:181:GLY:HA3	4:C:1390:GOL:H32	2.02	0.42
1:B:147:LYS:NZ	5:B:2207:HOH:O	2.34	0.42
1:C:25:VAL:O	1:C:350:MET:HA	2.20	0.42
1:C:59:ALA:HB2	1:C:94:LEU:HD21	2.02	0.42
1:A:233:ARG:NH2	4:A:1390:GOL:C3	2.80	0.41
1:C:148:GLN:CG	4:C:1392:GOL:O1	2.67	0.41
1:A:224:ARG:NH2	4:A:1390:GOL:O1	2.53	0.41
1:D:22:TYR:CZ	1:D:342:LYS:HG2	2.55	0.41
1:C:366:GLN:O	1:C:368:LEU:HD23	2.19	0.41
1:D:47:ASP:OD1	1:D:47:ASP:C	2.59	0.41
1:B:105:ARG:HD2	5:B:2147:HOH:O	2.20	0.41
1:A:218:HIS:O	4:A:1391:GOL:O1	2.39	0.41
1:B:124:PRO:HD2	1:B:125:PRO:HD2	2.03	0.41
1:B:141:TYR:CE1	1:B:179:SER:HB2	2.55	0.41
1:C:84:LYS:NZ	1:C:131:GLY:O	2.49	0.41
1:C:261:PHE:HB3	1:C:356:LEU:HD13	2.02	0.41
1:B:197:HIS:HD2	5:B:2215:HOH:O	2.03	0.41
1:A:335[B]:LYS:HE2	5:A:2402:HOH:O	2.21	0.41
1:D:59:ALA:HA	5:D:2022:HOH:O	2.20	0.41
1:D:44:ASP:H	1:D:79:MET:HE2	1.85	0.40
1:D:61:ILE:HD12	1:D:101:PHE:CZ	2.57	0.40
1:B:91:LYS:HD2	5:B:2128:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:TRP:O	1:D:141:TYR:HA	2.22	0.40
1:A:210:GLY:O	1:A:231:PRO:CG	2.69	0.40
1:C:225:GLY:HA2	1:C:313:GLY:HA3	2.03	0.40
1:A:22:TYR:CZ	1:A:342:LYS:HG2	2.56	0.40
1:A:283:ILE:HA	1:A:284:PRO:HD3	1.98	0.40
1:D:230:SER:HA	1:D:231:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/362 (102%)	358 (97%)	8 (2%)	2 (0%)	32	16
1	B	366/362 (101%)	358 (98%)	7 (2%)	1 (0%)	44	29
1	C	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
1	D	362/362 (100%)	352 (97%)	9 (2%)	1 (0%)	44	29
All	All	1453/1448 (100%)	1415 (97%)	34 (2%)	4 (0%)	44	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	GLY
1	D	365	GLY
1	A	145	ARG
1	B	365	GLY

### 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	309/302 (102%)	303 (98%)	6 (2%)	62	47
1	B	307/302 (102%)	302 (98%)	5 (2%)	68	55
1	C	301/302 (100%)	294 (98%)	7 (2%)	56	39
1	D	305/302 (101%)	298 (98%)	7 (2%)	56	39
All	All	1222/1208 (101%)	1197 (98%)	25 (2%)	59	45

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	106	PHE
1	A	144	ARG
1	A	213	ARG
1	A	344	ARG
1	A	368	LEU
1	B	86	ARG
1	B	106	PHE
1	B	144	ARG
1	B	344	ARG
1	B	368	LEU
1	C	62	SER
1	C	106	PHE
1	C	145	ARG
1	C	224	ARG
1	C	244	MET
1	C	317	PRO
1	C	368	LEU
1	D	76	LEU
1	D	89	ASN
1	D	106	PHE
1	D	144	ARG
1	D	160	GLU
1	D	164	GLU
1	D	286	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	89	ASN
1	A	130	HIS
1	A	148	GLN
1	A	197	HIS
1	A	315	GLN
1	B	85	ASN
1	B	89	ASN
1	B	196	GLN
1	B	197	HIS
1	C	85	ASN
1	C	87	ASN
1	C	148	GLN
1	D	63	ASN
1	D	85	ASN
1	D	89	ASN
1	D	130	HIS
1	D	171	GLN
1	D	345	GLN

### 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 ⓘ

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1383	1,2	14,14,15	0.65	0	15,19,21	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1384	2	14,14,15	0.62	0	15,19,21	0.68	0
2	NAG	B	1383	1,2	14,14,15	0.81	1 (7%)	15,19,21	0.94	0
2	NAG	B	1384	2	14,14,15	0.58	0	15,19,21	0.70	0
2	NAG	C	1383	1,2	14,14,15	0.45	0	15,19,21	0.95	1 (6%)
2	NAG	C	1384	2	14,14,15	0.49	0	15,19,21	0.66	0
2	NAG	D	1383	1,2	14,14,15	0.57	0	15,19,21	0.73	1 (6%)
2	NAG	D	1384	2	14,14,15	0.53	0	15,19,21	0.75	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	1383	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1384	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1383	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1384	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1383	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1384	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1383	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1384	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	B	1383	NAG	C1-C2	2.40	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1383	NAG	C2-N2-C7	-2.66	119.07	122.94
2	A	1383	NAG	C2-N2-C7	-2.22	119.71	122.94
2	D	1384	NAG	C2-N2-C7	-2.12	119.84	122.94
2	D	1383	NAG	C2-N2-C7	-2.09	119.90	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1383	NAG	3	0
2	B	1384	NAG	1	0

## 5.6 Ligand geometry

24 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	SO4	A	1385	-	4,4,4	0.33	0	6,6,6	0.18	0
4	GOL	A	1386	-	5,5,5	0.20	0	5,5,5	0.24	0
4	GOL	A	1387	-	5,5,5	0.38	0	5,5,5	0.18	0
4	GOL	A	1388	-	5,5,5	0.27	0	5,5,5	0.48	0
4	GOL	A	1389	-	5,5,5	0.35	0	5,5,5	0.49	0
4	GOL	A	1390	-	5,5,5	0.28	0	5,5,5	0.31	0
4	GOL	A	1391	-	5,5,5	0.31	0	5,5,5	0.39	0
3	SO4	B	1385	-	4,4,4	0.38	0	6,6,6	0.22	0
3	SO4	B	1386	-	4,4,4	0.40	0	6,6,6	0.46	0
3	SO4	B	1387	-	4,4,4	0.37	0	6,6,6	0.20	0
3	SO4	B	1388	-	4,4,4	0.29	0	6,6,6	0.32	0
4	GOL	B	1389	-	5,5,5	0.38	0	5,5,5	0.25	0
4	GOL	B	1390	-	5,5,5	0.22	0	5,5,5	0.26	0
3	SO4	C	1385	-	4,4,4	0.26	0	6,6,6	0.24	0
3	SO4	C	1386	-	4,4,4	0.24	0	6,6,6	0.23	0
3	SO4	C	1387	-	4,4,4	0.44	0	6,6,6	0.11	0
4	GOL	C	1388	-	5,5,5	0.35	0	5,5,5	0.52	0
4	GOL	C	1389	-	5,5,5	0.43	0	5,5,5	0.37	0
4	GOL	C	1390	-	5,5,5	0.16	0	5,5,5	0.33	0
4	GOL	C	1391	-	5,5,5	0.37	0	5,5,5	0.20	0
4	GOL	C	1392	-	5,5,5	0.22	0	5,5,5	0.45	0
4	GOL	D	1385	-	5,5,5	0.46	0	5,5,5	0.15	0
4	GOL	D	1386	-	5,5,5	0.30	0	5,5,5	0.34	0
4	GOL	D	1387	-	5,5,5	0.28	0	5,5,5	0.33	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	SO4	A	1385	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1386	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1387	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1388	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1389	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1390	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1391	-	-	0/4/4/4	0/0/0/0
3	SO4	B	1385	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1386	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1387	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1388	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1389	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1390	-	-	0/4/4/4	0/0/0/0
3	SO4	C	1385	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1386	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1387	-	-	0/0/0/0	0/0/0/0
4	GOL	C	1388	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1389	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1390	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1391	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1392	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1385	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1386	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1387	-	-	0/4/4/4	0/0/0/0

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.

16 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1386	GOL	1	0
4	A	1387	GOL	1	0
4	A	1388	GOL	11	0
4	A	1389	GOL	1	0
4	A	1390	GOL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1391	GOL	4	0
4	B	1389	GOL	5	0
4	B	1390	GOL	6	0
4	C	1388	GOL	2	0
4	C	1389	GOL	12	0
4	C	1390	GOL	14	0
4	C	1391	GOL	2	0
4	C	1392	GOL	9	0
4	D	1385	GOL	2	0
4	D	1386	GOL	2	0
4	D	1387	GOL	5	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 ⓘ

### 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	362/362 (100%)	-0.18	15 (4%) 38 36	14, 23, 45, 57	4 (1%)
1	B	362/362 (100%)	-0.24	12 (3%) 47 45	13, 24, 41, 64	2 (0%)
1	C	359/362 (99%)	0.11	24 (6%) 19 18	17, 33, 54, 70	3 (0%)
1	D	360/362 (99%)	0.51	43 (11%) 5 5	16, 37, 63, 76	7 (1%)
All	All	1443/1448 (99%)	0.05	94 (6%) 20 19	13, 28, 56, 76	16 (1%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	168	GLY	7.4
1	C	365	GLY	6.2
1	D	365	GLY	5.5
1	C	383	THR	5.3
1	C	104	GLN	5.1
1	D	165	ALA	5.1
1	D	63	ASN	4.9
1	C	99	TRP	4.7
1	D	71	TRP	4.6
1	D	65[A]	HIS	4.5
1	D	89	ASN	4.4
1	C	367	ASP	4.3
1	C	86	ARG	4.2
1	C	89	ASN	4.2
1	D	169	LYS	4.2
1	D	170	LYS	4.0
1	D	88	PRO	4.0
1	A	365	GLY	4.0
1	D	129	THR	3.9
1	D	144	ARG	3.9
1	D	99	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	368	LEU	3.7
1	B	365	GLY	3.7
1	B	366	GLN	3.7
1	C	103	SER	3.6
1	A	166[A]	GLN	3.6
1	B	166	GLN	3.5
1	D	86	ARG	3.4
1	C	368	LEU	3.4
1	D	367	ASP	3.3
1	B	383	THR	3.3
1	C	102	GLY	3.2
1	A	167	PRO	3.2
1	A	104	GLN	3.2
1	A	209	HIS	3.2
1	C	366	GLN	3.1
1	D	382	ALA	3.1
1	A	86	ARG	3.0
1	D	66	ILE	3.0
1	D	304[A]	ARG	3.0
1	D	366	GLN	2.9
1	C	364	CYS	2.9
1	C	169	LYS	2.9
1	D	112	ASN	2.9
1	D	103	SER	2.9
1	A	368	LEU	2.8
1	B	382	ALA	2.8
1	C	129	THR	2.7
1	C	88	PRO	2.7
1	B	367	ASP	2.7
1	D	59	ALA	2.7
1	C	65	HIS	2.7
1	B	104	GLN	2.6
1	C	49	PHE	2.6
1	A	367	ASP	2.6
1	D	209	HIS	2.6
1	D	75	THR	2.6
1	D	114	GLN	2.6
1	D	61	ILE	2.5
1	A	102	GLY	2.5
1	A	383	THR	2.5
1	A	212	TRP	2.5
1	D	83	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	125	PRO	2.4
1	A	88	PRO	2.4
1	C	63	ASN	2.4
1	C	100	ASN	2.4
1	A	231	PRO	2.4
1	D	383	THR	2.4
1	C	196	GLN	2.3
1	D	85	ASN	2.3
1	D	100	ASN	2.3
1	C	71	TRP	2.3
1	D	102	GLY	2.3
1	B	86	ARG	2.3
1	D	49	PHE	2.3
1	D	121	LYS	2.3
1	A	89	ASN	2.2
1	C	163	LYS	2.2
1	B	89	ASN	2.2
1	C	304	ARG	2.2
1	B	88	PRO	2.2
1	B	167	PRO	2.2
1	D	117	ARG	2.1
1	D	381	ALA	2.1
1	D	364	CYS	2.1
1	D	162	ILE	2.1
1	D	155	LYS	2.1
1	D	286	ARG	2.1
1	C	101	PHE	2.1
1	D	34	TYR	2.0
1	A	114	GLN	2.0
1	D	38	ASP	2.0
1	B	102	GLY	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	NAG	C	1383	14/15	0.83	0.20	1.11	54,56,62,65	0
2	NAG	A	1383	14/15	0.90	0.12	0.14	36,44,52,53	0
2	NAG	D	1383	14/15	0.79	0.21	-0.04	65,67,71,73	0
2	NAG	B	1383	14/15	0.90	0.11	-0.23	29,34,42,50	0
2	NAG	B	1384	14/15	0.84	0.24	-	46,48,55,59	0
2	NAG	A	1384	14/15	0.85	0.35	-	56,59,60,61	0
2	NAG	D	1384	14/15	0.77	0.39	-	75,76,77,79	0
2	NAG	C	1384	14/15	0.80	0.43	-	68,71,72,73	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	GOL	C	1389	6/6	0.72	0.56	27.75	38,55,60,66	0
3	SO4	B	1385	5/5	0.92	0.19	9.33	63,64,65,65	0
4	GOL	A	1388	6/6	0.82	0.37	6.37	52,54,56,61	0
4	GOL	C	1392	6/6	0.71	0.39	5.99	70,70,71,71	0
4	GOL	A	1390	6/6	0.73	0.35	5.12	59,63,65,65	0
4	GOL	C	1388	6/6	0.84	0.18	4.85	39,49,52,56	0
4	GOL	A	1387	6/6	0.80	0.24	4.57	62,64,64,65	0
4	GOL	D	1385	6/6	0.89	0.22	3.80	36,45,46,46	0
4	GOL	D	1387	6/6	0.75	0.34	3.72	61,62,63,66	0
4	GOL	B	1389	6/6	0.80	0.16	3.47	54,55,55,56	0
4	GOL	A	1389	6/6	0.84	0.21	3.32	35,41,42,46	0
4	GOL	A	1391	6/6	0.89	0.23	3.11	35,42,45,46	0
4	GOL	C	1390	6/6	0.81	0.29	2.83	60,62,62,62	0
3	SO4	B	1386	5/5	0.88	0.15	1.77	48,51,52,53	0
4	GOL	D	1386	6/6	0.77	0.21	1.73	50,51,51,54	0
4	GOL	A	1386	6/6	0.86	0.20	1.56	23,41,43,46	0
3	SO4	C	1386	5/5	0.97	0.10	0.45	53,53,54,56	0
3	SO4	B	1388	5/5	0.97	0.11	0.23	48,48,50,50	0
3	SO4	C	1385	5/5	0.96	0.09	-1.05	55,57,58,58	0
3	SO4	B	1387	5/5	0.89	0.21	-	75,75,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	1387	5/5	0.95	0.32	-	76,77,77,78	0
4	GOL	B	1390	6/6	0.65	0.31	-	67,69,69,71	0
3	SO4	A	1385	5/5	0.91	0.17	-	70,71,72,73	0
4	GOL	C	1391	6/6	0.84	0.20	-	64,65,65,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.