



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:57 pm GMT

PDB ID : 3LB6  
Title : The structure of IL-13 in complex with IL-13Ralpha2  
Authors : Lupardus, P.J.; Garcia, K.C.; Birnbaum, M.E.  
Deposited on : 2010-01-07  
Resolution : 3.05 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.

---

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

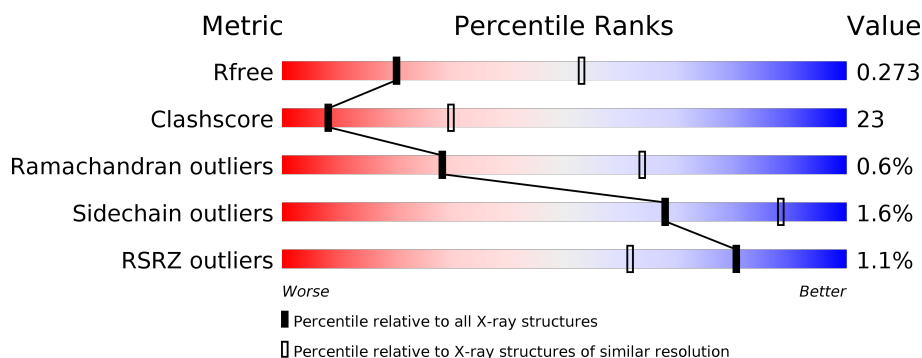
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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	132	<div> <div> <div></div> <div>58%</div> <div>23%</div> <div>17%</div> </div> <div> <div></div> <div>39%</div> <div>26%</div> <div>34%</div> </div> </div>
2	C	380	<div> <div>2%</div> <div>39%</div> <div>26%</div> <div>34%</div> </div> <div> <div></div> <div>61%</div> <div>21%</div> <div>17%</div> </div>
3	B	132	<div> <div></div> <div>61%</div> <div>21%</div> <div>17%</div> </div> <div> <div></div> <div>46%</div> <div>28%</div> <div>25%</div> </div>
4	D	380	<div> <div></div> <div>46%</div> <div>28%</div> <div>25%</div> </div> <div> <div></div> <div>61%</div> <div>21%</div> <div>17%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6088 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 Interleukin-13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			830	526	145	152	7			

- Molecule 2 is a protein called Interleukin-13 receptor subunit alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	252	Total	C	N	O	S	0	0	0
			2047	1343	315	379	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	151	GLN	ARG	engineered	UNP A8K7E2

- Molecule 3 is a protein called Interleukin-13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	109	Total	C	N	O	S	0	0	0
			840	533	147	153	7			

- Molecule 4 is a protein called Interleukin-13 receptor subunit alpha-2.

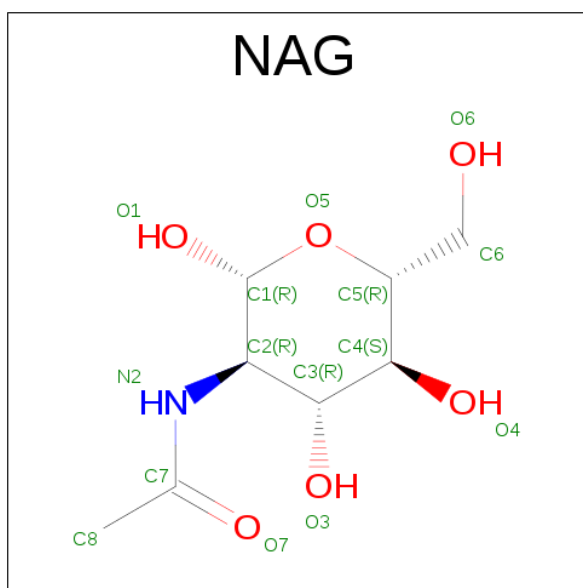
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	286	Total	C	N	O	S	5	0	0
			2310	1501	362	435	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	151	GLN	ARG	engineered	UNP A8K7E2

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

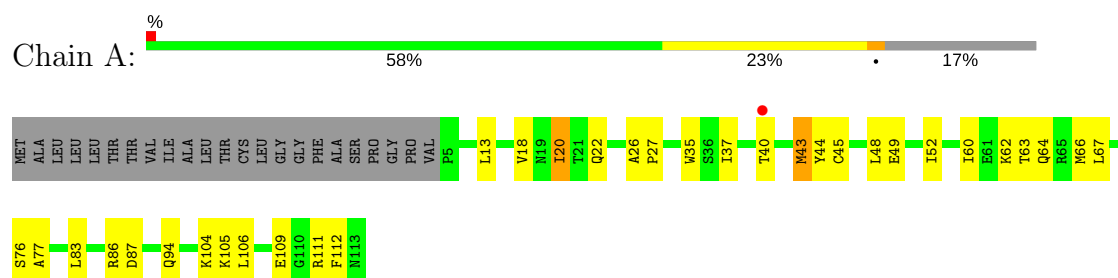
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	O	0	0
			7	7		
7	C	4	Total	O	0	0
			4	4		
7	B	4	Total	O	0	0
			4	4		
7	D	16	Total	O	0	0
			16	16		

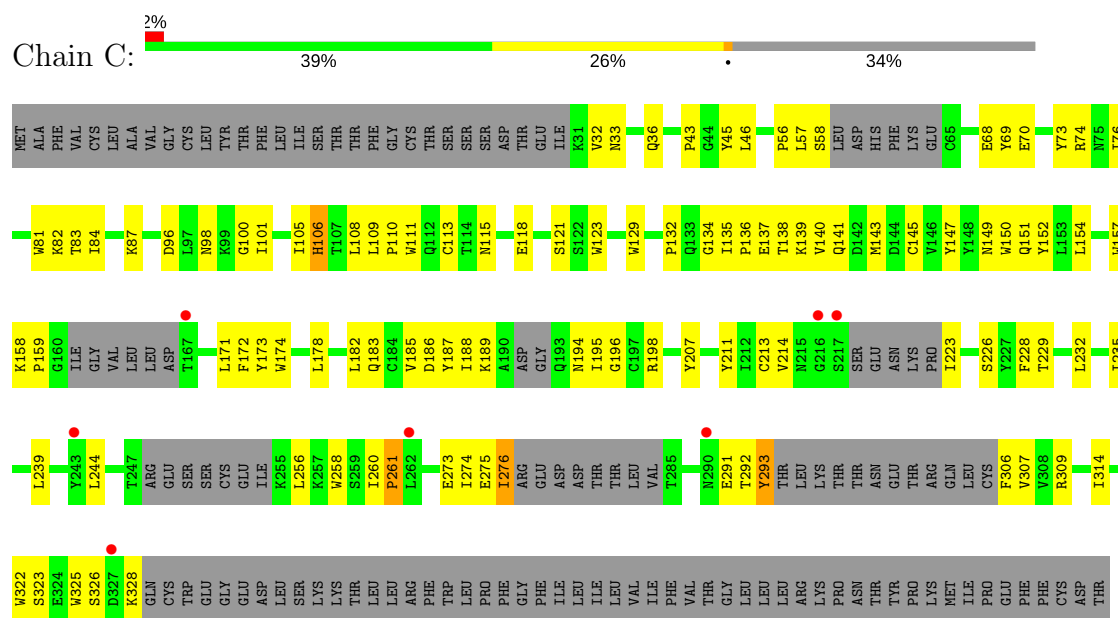
### 3 Residue-property plots

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.

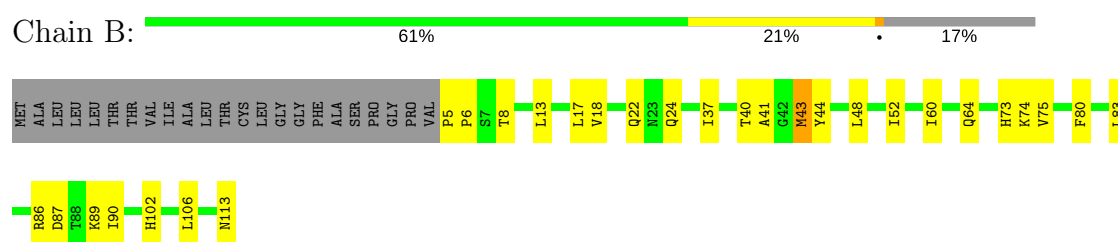
#### • Molecule 1: Interleukin-13



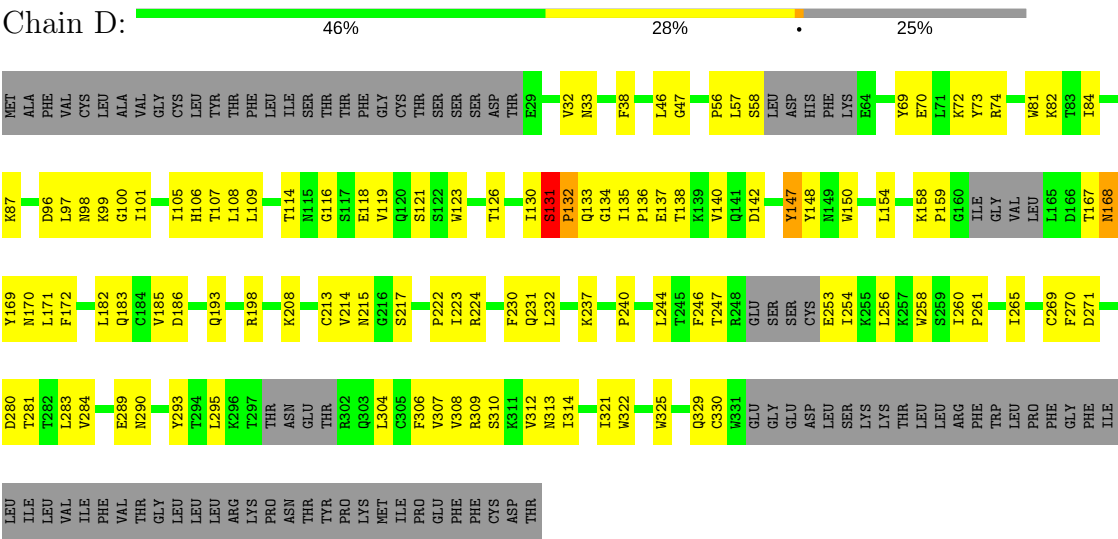
#### • Molecule 2: Interleukin-13 receptor subunit alpha-2



#### • Molecule 3: Interleukin-13



● Molecule 4: Interleukin-13 receptor subunit alpha-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.37Å 86.57Å 166.79Å 90.00° 96.77° 90.00°	Depositor
Resolution (Å)	82.80 – 3.05 82.81 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.2 (82.80-3.05) 100.0 (82.81-3.05)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.219 , 0.269 0.222 , 0.273	Depositor DCC
$R_{free}$ test set	1018 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.70% 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, MLY, NAG

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	0/844	0.71	1/1140 (0.1%)
2	C	0.49	1/2090 (0.0%)	0.63	0/2858
3	B	0.54	0/843	0.71	1/1138 (0.1%)
4	D	0.61	0/2357	0.72	1/3225 (0.0%)
All	All	0.55	1/6134 (0.0%)	0.69	3/8361 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	261	PRO	N-CD	6.21	1.56	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	MET	CB-CA-C	-5.66	99.09	110.40
4	D	131	SER	C-N-CD	-5.49	108.52	120.60
3	B	43	MET	CB-CA-C	-5.05	100.29	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	830	0	832	24	1
2	C	2047	0	1874	122	1
3	B	840	0	851	21	0
4	D	2310	0	2139	116	1
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	7	0	0	2	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
7	D	16	0	0	2	0
All	All	6088	0	5722	276	2

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 23.

All (276) 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)
4:D:167:THR:HG23	4:D:217:SER:O	1.21	1.30
2:C:140:VAL:HG21	2:C:157:TRP:CD1	1.77	1.19
2:C:292:THR:HG22	2:C:293:TYR:H	1.26	1.00
4:D:134:GLY:O	4:D:224:ARG:NH2	1.94	1.00
4:D:167:THR:CG2	4:D:217:SER:O	2.08	0.99
4:D:280:ASP:O	4:D:281:THR:HG22	1.67	0.93
3:B:43:MET:HG3	3:B:44:TYR:N	1.84	0.93
4:D:169:TYR:HE2	4:D:193:GLN:HE21	1.17	0.92
2:C:292:THR:HG22	2:C:293:TYR:N	1.84	0.91
4:D:148:TYR:CE2	4:D:154:LEU:HD12	2.05	0.91
3:B:60:ILE:O	3:B:64:GLN:HG3	1.71	0.90
2:C:140:VAL:HG21	2:C:157:TRP:HD1	1.41	0.86
4:D:247:THR:O	4:D:254:ILE:HG13	1.79	0.83
4:D:140:VAL:CG1	4:D:169:TYR:CE1	2.63	0.81
4:D:169:TYR:HE2	4:D:193:GLN:NE2	1.79	0.80
4:D:97:LEU:HD13	4:D:130:ILE:HD11	1.63	0.80
4:D:290:ASN:OD1	7:D:397:HOH:O	1.99	0.80
2:C:244:LEU:HB3	2:C:306:PHE:CZ	2.17	0.80
2:C:276:ILE:HG22	2:C:306:PHE:HA	1.64	0.80
2:C:76:ILE:HD12	2:C:100:GLY:HA3	1.64	0.80
2:C:135:ILE:O	2:C:138:THR:HG22	1.82	0.79
2:C:69:TYR:HB3	2:C:105:ILE:HD11	1.66	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:87:ASP:HB3	4:D:87:LYS:HE2	1.67	0.77
2:C:275:GLU:O	2:C:275:GLU:HG2	1.82	0.77
4:D:96:ASP:OD2	4:D:98:ASN:HB2	1.84	0.76
2:C:140:VAL:CG2	2:C:157:TRP:CD1	2.64	0.76
2:C:140:VAL:HG23	2:C:158:LYS:O	1.86	0.76
2:C:185:VAL:HG23	2:C:186:ASP:N	2.01	0.75
2:C:292:THR:CG2	2:C:293:TYR:H	1.99	0.75
2:C:260:ILE:HD12	2:C:261:PRO:O	1.87	0.75
4:D:280:ASP:O	4:D:281:THR:CG2	2.35	0.75
1:A:112:PHE:HB3	7:A:119:HOH:O	1.88	0.74
1:A:94:GLN:NE2	7:A:120:HOH:O	2.19	0.74
2:C:137:GLU:H	2:C:139:MLY:CG	2.01	0.73
3:B:43:MET:CG	3:B:44:TYR:N	2.52	0.73
2:C:174:TRP:HA	2:C:178:LEU:HD12	1.72	0.72
2:C:185:VAL:HG23	2:C:186:ASP:H	1.55	0.71
4:D:97:LEU:HB3	4:D:130:ILE:HD12	1.72	0.71
4:D:280:ASP:C	4:D:281:THR:CG2	2.60	0.70
2:C:137:GLU:H	2:C:139:MLY:HG3	1.56	0.70
2:C:273:GLU:OE1	2:C:309:ARG:NH2	2.24	0.69
4:D:309:ARG:HD3	4:D:325:TRP:CE2	2.28	0.69
4:D:38:PHE:CE2	4:D:126:THR:HG22	2.28	0.69
2:C:293:TYR:HD2	2:C:293:TYR:O	1.76	0.67
4:D:170:ASN:HB3	4:D:172:PHE:HE1	1.58	0.67
3:B:102:HIS:NE2	3:B:106:LEU:HD11	2.09	0.67
2:C:32:VAL:HG13	2:C:121:SER:HB3	1.77	0.67
4:D:154:LEU:CD2	4:D:198:ARG:HG2	2.24	0.66
2:C:57:LEU:O	2:C:58:SER:HB2	1.95	0.66
2:C:226:SER:HB3	2:C:228:PHE:CE1	2.31	0.66
2:C:276:ILE:HG21	2:C:306:PHE:HB2	1.76	0.66
4:D:254:ILE:CG2	4:D:295:LEU:HB3	2.26	0.65
1:A:43:MET:HG3	1:A:44:TYR:N	2.10	0.65
2:C:110:PRO:HD2	2:C:113:CYS:SG	2.37	0.65
4:D:74:ARG:NH1	4:D:81:TRP:NE1	2.44	0.65
4:D:131:SER:O	4:D:132:PRO:C	2.33	0.65
2:C:68:GLU:HB2	2:C:108:LEU:HB3	1.79	0.64
2:C:140:VAL:CG2	2:C:157:TRP:HD1	2.07	0.64
2:C:140:VAL:CG2	2:C:158:LYS:O	2.46	0.64
4:D:289:GLU:O	7:D:397:HOH:O	2.15	0.64
1:A:109:GLU:OE1	1:A:111:ARG:HD2	1.98	0.64
2:C:106:HIS:ND1	2:C:106:HIS:O	2.30	0.63
4:D:32:VAL:HG13	4:D:121:SER:HB3	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CD2	1:A:86:ARG:HG2	2.35	0.62
2:C:309:ARG:HD2	2:C:323:SER:O	1.99	0.62
1:A:37:ILE:HG22	1:A:83:LEU:HD13	1.81	0.62
4:D:253:GLU:HA	4:D:295:LEU:O	1.99	0.62
4:D:140:VAL:HG12	4:D:169:TYR:CE1	2.34	0.62
4:D:131:SER:O	4:D:132:PRO:O	2.18	0.61
2:C:134:GLY:HA3	2:C:223:ILE:HA	1.81	0.61
2:C:275:GLU:CG	2:C:275:GLU:O	2.49	0.61
2:C:45:TYR:O	2:C:46:LEU:HB2	2.01	0.61
4:D:32:VAL:HG22	4:D:33:ASN:N	2.14	0.61
3:B:18:VAL:HG21	4:D:314:ILE:HD12	1.83	0.61
2:C:171:LEU:HD23	2:C:172:PHE:N	2.16	0.60
1:A:87:ASP:HB3	2:C:87:LYS:HE2	1.83	0.60
2:C:256:LEU:C	2:C:256:LEU:HD12	2.23	0.59
2:C:137:GLU:N	2:C:139:MLY:HG3	2.18	0.59
4:D:246:PHE:CE1	4:D:256:LEU:HD12	2.37	0.59
2:C:309:ARG:HG3	2:C:323:SER:O	2.02	0.59
2:C:109:LEU:O	2:C:118:GLU:HG3	2.03	0.59
4:D:100:GLY:C	4:D:101:ILE:HD12	2.22	0.59
4:D:101:ILE:N	4:D:101:ILE:HD12	2.17	0.59
4:D:167:THR:HG22	4:D:168:ASN:N	2.17	0.59
1:A:62:LYS:HD3	1:A:66:MET:HE3	1.85	0.58
2:C:274:ILE:HG23	2:C:274:ILE:O	2.03	0.58
2:C:135:ILE:O	2:C:138:THR:CG2	2.52	0.58
4:D:133:GLN:O	4:D:133:GLN:HG3	2.04	0.58
1:A:13:LEU:HD12	1:A:13:LEU:O	2.04	0.57
2:C:32:VAL:HG22	2:C:33:ASN:N	2.19	0.57
2:C:185:VAL:CG2	2:C:186:ASP:H	2.18	0.57
3:B:13:LEU:HD12	3:B:13:LEU:O	2.04	0.57
2:C:232:LEU:O	2:C:235:ILE:HG22	2.05	0.57
2:C:76:ILE:HD12	2:C:100:GLY:CA	2.33	0.57
4:D:172:PHE:CE2	4:D:183:GLN:HB2	2.40	0.57
4:D:280:ASP:C	4:D:281:THR:HG23	2.23	0.57
1:A:62:LYS:HD3	1:A:66:MET:CE	2.34	0.57
2:C:188:ILE:HB	2:C:196:GLY:HA3	1.87	0.56
4:D:46:LEU:HD23	4:D:213:CYS:N	2.19	0.56
3:B:37:ILE:HG22	3:B:83:LEU:HD13	1.87	0.56
4:D:56:PRO:HG2	4:D:107:THR:HG21	1.85	0.56
1:A:18:VAL:O	1:A:22:GLN:HG2	2.05	0.56
2:C:185:VAL:CG2	2:C:186:ASP:N	2.68	0.56
2:C:309:ARG:CG	2:C:323:SER:O	2.54	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:271:ASP:OD2	4:D:313:ASN:HB3	2.06	0.56
4:D:140:VAL:HG11	4:D:169:TYR:CD1	2.41	0.56
2:C:171:LEU:HD23	2:C:171:LEU:C	2.26	0.56
4:D:106:HIS:CE1	4:D:123:TRP:CH2	2.94	0.56
4:D:72:LYS:HA	4:D:82:MLY:O	2.06	0.55
4:D:256:LEU:HD21	4:D:306:PHE:CD1	2.41	0.55
4:D:185:VAL:HG23	4:D:186:ASP:H	1.70	0.55
2:C:256:LEU:HD13	2:C:306:PHE:CZ	2.42	0.55
3:B:18:VAL:O	3:B:22:GLN:HG2	2.07	0.55
2:C:276:ILE:CG2	2:C:306:PHE:HA	2.35	0.54
2:C:83:THR:O	2:C:84:ILE:CG2	2.55	0.54
2:C:292:THR:CG2	2:C:293:TYR:N	2.55	0.54
2:C:293:TYR:CD2	2:C:293:TYR:O	2.60	0.54
4:D:244:LEU:HB3	4:D:306:PHE:CZ	2.43	0.54
1:A:40:THR:O	1:A:43:MET:HB3	2.08	0.53
4:D:244:LEU:HD22	4:D:258:TRP:HB2	1.91	0.53
3:B:24:GLN:O	3:B:24:GLN:HG3	2.09	0.53
2:C:256:LEU:O	2:C:292:THR:HA	2.09	0.53
4:D:148:TYR:CD2	4:D:154:LEU:HD12	2.44	0.53
2:C:70:GLU:HB3	2:C:106:HIS:CE1	2.44	0.52
2:C:187:TYR:HB2	2:C:189:LYS:HE3	1.90	0.52
2:C:256:LEU:O	2:C:256:LEU:HD12	2.10	0.52
1:A:45:CYS:O	1:A:49:GLU:HG3	2.09	0.52
2:C:36:GLN:OE1	2:C:57:LEU:HD11	2.09	0.52
2:C:106:HIS:CD2	2:C:123:TRP:CZ2	2.98	0.52
4:D:135:ILE:HB	4:D:136:PRO:HD2	1.91	0.52
4:D:170:ASN:HB3	4:D:172:PHE:CE1	2.43	0.52
3:B:40:THR:O	3:B:43:MET:HB3	2.11	0.51
4:D:171:LEU:HD23	4:D:172:PHE:N	2.25	0.51
4:D:140:VAL:CG1	4:D:169:TYR:CD1	2.94	0.51
2:C:140:VAL:HG22	2:C:141:GLN:N	2.26	0.51
1:A:104:LYS:HE2	2:C:314:ILE:O	2.11	0.51
4:D:171:LEU:C	4:D:171:LEU:HD23	2.30	0.51
4:D:307:VAL:HG12	4:D:308:VAL:N	2.27	0.50
2:C:96:ASP:OD2	2:C:98:ASN:HB2	2.11	0.50
2:C:309:ARG:CD	2:C:323:SER:O	2.60	0.50
4:D:142:ASP:OD2	4:D:158:LYS:HD2	2.11	0.50
4:D:260:ILE:HB	4:D:261:PRO:HD2	1.93	0.50
1:A:48:LEU:HD13	1:A:67:LEU:HB2	1.94	0.50
2:C:226:SER:HB3	2:C:228:PHE:CZ	2.47	0.50
2:C:189:LYS:HD3	2:C:194:ASN:OD1	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:HIS:CD2	2:C:123:TRP:CH2	3.00	0.49
3:B:73:HIS:CE1	3:B:75:VAL:HG22	2.48	0.49
4:D:304:LEU:O	4:D:330:CYS:HA	2.12	0.49
4:D:154:LEU:HD21	4:D:198:ARG:HG2	1.94	0.49
4:D:170:ASN:HB2	4:D:215:ASN:HB2	1.94	0.49
4:D:283:LEU:HD21	4:D:295:LEU:HD11	1.95	0.49
2:C:139:MLY:HH22	2:C:139:MLY:HD2	1.58	0.48
2:C:101:ILE:HD12	2:C:101:ILE:N	2.28	0.48
1:A:62:LYS:O	1:A:63:THR:C	2.51	0.48
2:C:73:TYR:HE2	2:C:82:LYS:HD3	1.77	0.48
2:C:154:LEU:HD11	2:C:198:ARG:HG2	1.95	0.48
4:D:185:VAL:HG23	4:D:186:ASP:N	2.29	0.48
2:C:73:TYR:CE2	2:C:82:LYS:HB2	2.48	0.48
2:C:195:ILE:HD12	2:C:195:ILE:C	2.34	0.48
2:C:258:TRP:CZ2	2:C:291:GLU:HA	2.49	0.48
1:A:60:ILE:O	1:A:64:GLN:HG3	2.12	0.48
3:B:80:PHE:CD1	3:B:86:ARG:HD2	2.49	0.48
2:C:145:CYS:C	2:C:235:ILE:HD11	2.35	0.48
4:D:131:SER:C	4:D:132:PRO:O	2.52	0.47
4:D:138:THR:HB	4:D:223:ILE:HB	1.96	0.47
4:D:114:THR:C	4:D:116:GLY:H	2.16	0.47
1:A:37:ILE:HG22	1:A:83:LEU:CD1	2.44	0.47
4:D:254:ILE:HG22	4:D:295:LEU:HB3	1.95	0.47
4:D:167:THR:CG2	4:D:168:ASN:N	2.78	0.47
2:C:145:CYS:CB	2:C:235:ILE:HD11	2.45	0.47
4:D:217:SER:HA	4:D:222:PRO:HA	1.96	0.47
4:D:135:ILE:C	4:D:137:GLU:H	2.18	0.46
3:B:40:THR:HB	3:B:41:ALA:H	1.55	0.46
2:C:276:ILE:HG21	2:C:306:PHE:CB	2.42	0.46
3:B:87:ASP:CB	4:D:87:LYS:HE2	2.43	0.46
2:C:273:GLU:HB2	2:C:322:TRP:CH2	2.49	0.46
4:D:138:THR:CB	4:D:223:ILE:HB	2.46	0.46
2:C:111:TRP:O	2:C:115:ASN:N	2.49	0.46
2:C:43:PRO:HB2	2:C:45:TYR:CD1	2.51	0.46
2:C:136:PRO:HA	2:C:139:MLY:HG3	1.98	0.46
4:D:32:VAL:CG2	4:D:33:ASN:N	2.78	0.46
4:D:57:LEU:O	4:D:58:SER:CB	2.64	0.46
4:D:97:LEU:HB3	4:D:130:ILE:CD1	2.42	0.46
2:C:276:ILE:CG2	2:C:306:PHE:HB2	2.45	0.45
2:C:84:ILE:HD12	2:C:84:ILE:C	2.37	0.45
4:D:132:PRO:HG2	4:D:132:PRO:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:CYS:HB3	2:C:235:ILE:HD11	1.98	0.45
2:C:244:LEU:HD11	2:C:326:SER:OG	2.16	0.45
4:D:99:MLY:HH22	4:D:99:MLY:HD3	1.74	0.45
2:C:45:TYR:HB3	2:C:174:TRP:CE3	2.51	0.45
4:D:69:TYR:HB3	4:D:105:ILE:HD11	1.98	0.45
4:D:271:ASP:CG	4:D:313:ASN:HB3	2.37	0.45
2:C:244:LEU:HD22	2:C:258:TRP:HB2	1.99	0.45
2:C:83:THR:O	2:C:84:ILE:HG22	2.16	0.45
2:C:147:TYR:HB2	2:C:235:ILE:HG23	1.99	0.45
2:C:314:ILE:HG13	2:C:314:ILE:O	2.17	0.45
4:D:244:LEU:HD22	4:D:258:TRP:CB	2.46	0.45
2:C:174:TRP:CD1	2:C:178:LEU:HB2	2.52	0.44
2:C:143:MET:HG2	2:C:228:PHE:CE2	2.52	0.44
2:C:274:ILE:HG13	2:C:307:VAL:O	2.17	0.44
4:D:310:SER:O	4:D:322:TRP:HE3	2.00	0.44
1:A:52:ILE:HG23	1:A:77:ALA:HA	1.99	0.44
2:C:129:TRP:CH2	2:C:132:PRO:CG	3.01	0.44
2:C:244:LEU:HB3	2:C:306:PHE:HZ	1.79	0.44
1:A:43:MET:CG	1:A:44:TYR:N	2.78	0.44
4:D:240:PRO:O	4:D:261:PRO:HB3	2.16	0.44
4:D:284:VAL:HG11	4:D:293:TYR:OH	2.18	0.44
4:D:269:CYS:O	4:D:312:VAL:HA	2.18	0.44
4:D:310:SER:O	4:D:322:TRP:CE3	2.71	0.44
4:D:246:PHE:HE2	4:D:329:GLN:C	2.21	0.44
4:D:109:LEU:HB2	4:D:119:VAL:HG13	2.00	0.44
4:D:154:LEU:CD2	4:D:198:ARG:CG	2.95	0.44
4:D:82:MLY:HD3	4:D:82:MLY:HH22	1.74	0.44
1:A:20:ILE:O	1:A:20:ILE:HG13	2.18	0.43
2:C:100:GLY:HA2	2:C:129:TRP:HD1	1.83	0.43
2:C:244:LEU:N	2:C:244:LEU:HD23	2.33	0.43
2:C:307:VAL:HG12	2:C:328:LYS:HA	1.99	0.43
4:D:246:PHE:HE2	4:D:329:GLN:O	2.01	0.43
2:C:228:PHE:N	2:C:228:PHE:CD1	2.86	0.43
2:C:275:GLU:HB3	2:C:325:TRP:CH2	2.54	0.43
4:D:134:GLY:H	4:D:224:ARG:HE	1.64	0.43
1:A:106:LEU:HD22	1:A:111:ARG:HD3	2.00	0.43
2:C:33:ASN:O	2:C:56:PRO:HB3	2.18	0.43
2:C:136:PRO:O	2:C:137:GLU:CB	2.66	0.43
4:D:307:VAL:HG12	4:D:325:TRP:HE3	1.84	0.43
2:C:235:ILE:O	2:C:235:ILE:HG12	2.18	0.43
4:D:147:TYR:CD2	4:D:232:LEU:HB3	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:TRP:CZ2	2:C:132:PRO:HG3	2.54	0.42
2:C:151:GLN:HG2	2:C:152:TYR:CE1	2.54	0.42
2:C:158:LYS:HA	2:C:159:PRO:HD3	1.80	0.42
3:B:17:LEU:HA	3:B:17:LEU:HD23	1.79	0.42
2:C:83:THR:C	2:C:84:ILE:HG23	2.38	0.42
4:D:105:ILE:O	4:D:105:ILE:HG23	2.19	0.42
2:C:172:PHE:HA	2:C:182:LEU:O	2.19	0.42
2:C:76:ILE:HG13	2:C:76:ILE:H	1.67	0.42
4:D:260:ILE:HD12	4:D:261:PRO:O	2.19	0.42
4:D:96:ASP:OD2	4:D:98:ASN:N	2.45	0.42
3:B:48:LEU:O	3:B:52:ILE:HB	2.20	0.42
3:B:74:LYS:HG3	3:B:75:VAL:N	2.34	0.42
2:C:229:THR:HG23	2:C:229:THR:O	2.20	0.42
4:D:130:ILE:O	4:D:132:PRO:N	2.53	0.42
4:D:140:VAL:HG21	4:D:214:VAL:HG11	2.01	0.42
3:B:5:PRO:HB2	3:B:8:THR:HG23	2.01	0.42
2:C:173:TYR:HA	2:C:211:TYR:O	2.19	0.42
4:D:172:PHE:HA	4:D:182:LEU:O	2.20	0.42
4:D:47:GLY:HA2	4:D:97:LEU:HG	2.02	0.42
4:D:154:LEU:HD23	4:D:198:ARG:HA	2.01	0.41
3:B:89:MLY:HD2	3:B:89:MLY:HH23	1.73	0.41
4:D:265:ILE:CG2	4:D:270:PHE:CE1	3.03	0.41
4:D:73:TYR:CE2	4:D:82:MLY:HD3	2.55	0.41
4:D:74:ARG:HD3	4:D:81:TRP:CD2	2.55	0.41
2:C:188:ILE:HB	2:C:196:GLY:CA	2.50	0.41
4:D:158:LYS:HA	4:D:159:PRO:HD3	1.87	0.41
4:D:208:LYS:O	4:D:231:GLN:HG2	2.20	0.41
2:C:291:GLU:O	2:C:292:THR:OG1	2.33	0.41
1:A:105:LYS:HG3	2:C:207:TYR:CG	2.55	0.41
4:D:244:LEU:HD13	4:D:306:PHE:CE1	2.55	0.41
4:D:170:ASN:O	4:D:214:VAL:HA	2.21	0.41
2:C:140:VAL:HG11	2:C:214:VAL:HG11	2.02	0.41
4:D:237:LYS:HG3	4:D:322:TRP:O	2.20	0.41
2:C:138:THR:O	2:C:223:ILE:HD13	2.21	0.41
1:A:26:ALA:HB1	1:A:27:PRO:HD2	2.03	0.41
2:C:149:ASN:ND2	2:C:239:LEU:HD12	2.36	0.41
2:C:172:PHE:CE2	2:C:183:GLN:HB2	2.56	0.41
2:C:32:VAL:CG2	2:C:33:ASN:N	2.84	0.41
4:D:138:THR:OG1	4:D:224:ARG:N	2.47	0.41
4:D:283:LEU:HG	4:D:284:VAL:HG23	2.03	0.41
4:D:70:GLU:HB3	4:D:106:HIS:NE2	2.37	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:106:HIS:ND1	4:D:123:TRP:CH2	2.89	0.40
4:D:246:PHE:CZ	4:D:306:PHE:HD2	2.38	0.40
2:C:46:LEU:HD23	2:C:213:CYS:N	2.36	0.40
4:D:230:PHE:HE1	4:D:232:LEU:HD23	1.86	0.40
4:D:254:ILE:HG23	4:D:295:LEU:HB3	2.02	0.40
3:B:90:ILE:HG22	4:D:84:ILE:HG22	2.03	0.40
4:D:246:PHE:CE2	4:D:329:GLN:O	2.74	0.40
2:C:74:ARG:NH1	2:C:81:TRP:NE1	2.69	0.40

All (2) 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:76:SER:OG	4:D:118:GLU:OE1[4_555]	1.96	0.24
2:C:198:ARG:NH2	2:C:260:ILE:CD1[2_655]	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	107/132 (81%)	94 (88%)	12 (11%)	1 (1%)	20	55
2	C	234/380 (62%)	204 (87%)	30 (13%)	0	100	100
3	B	106/132 (80%)	94 (89%)	11 (10%)	1 (1%)	20	55
4	D	274/380 (72%)	240 (88%)	32 (12%)	2 (1%)	25	61
All	All	721/1024 (70%)	632 (88%)	85 (12%)	4 (1%)	28	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	131	SER

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
4	D	132	PRO
1	A	20	ILE
3	B	6	PRO

### 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	91/112 (81%)	91 (100%)	0	100	100
2	C	215/349 (62%)	211 (98%)	4 (2%)	62	85
3	B	92/111 (83%)	91 (99%)	1 (1%)	78	91
4	D	246/349 (70%)	241 (98%)	5 (2%)	60	85
All	All	644/921 (70%)	634 (98%)	10 (2%)	68	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	106	HIS
2	C	150	TRP
2	C	276	ILE
2	C	293	TYR
3	B	113	ASN
4	D	108	LEU
4	D	147	TYR
4	D	150	TRP
4	D	168	ASN
4	D	321	ILE

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	MLY	B	89	3	10,10,11	0.63	0	8,11,13	1.67	2 (25%)
2	MLY	C	104	2	10,10,11	0.89	1 (10%)	8,11,13	1.32	2 (25%)
2	MLY	C	139	2	10,10,11	0.76	0	8,11,13	1.10	1 (12%)
4	MLY	D	82	4	10,10,11	0.62	0	8,11,13	1.46	1 (12%)
4	MLY	D	99	4	10,10,11	0.74	0	8,11,13	1.50	2 (25%)

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	MLY	B	89	3	-	0/7/9/11	0/0/0/0
2	MLY	C	104	2	-	0/7/9/11	0/0/0/0
2	MLY	C	139	2	-	0/7/9/11	0/0/0/0
4	MLY	D	82	4	-	0/7/9/11	0/0/0/0
4	MLY	D	99	4	-	0/7/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	104	MLY	CA-C	2.31	1.53	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	99	MLY	CD-CE-NZ	-2.83	106.09	113.77
3	B	89	MLY	CD-CE-NZ	-2.69	106.47	113.77
4	D	82	MLY	CD-CE-NZ	-2.54	106.86	113.77
2	C	139	MLY	O-C-CA	-2.23	118.86	125.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	104	MLY	O-C-CA	-2.16	119.05	125.02
4	D	99	MLY	O-C-CA	-2.16	119.06	125.02
3	B	89	MLY	CB-CA-C	-2.15	108.11	111.65
2	C	104	MLY	CD-CE-NZ	-2.09	108.09	113.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	89	MLY	1	0
2	C	139	MLY	5	0
4	D	82	MLY	3	0
4	D	99	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	C	501	2	14,14,15	0.57	0	15,19,21	1.26	2 (13%)
5	NAG	D	501	4	14,14,15	0.54	0	15,19,21	1.12	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	501	2	-	0/6/23/26	0/1/1/1
5	NAG	D	501	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	NAG	C2-N2-C7	-2.32	119.56	122.94
5	C	501	NAG	C1-C2-N2	-2.15	106.81	110.49
5	C	501	NAG	C4-C3-C2	2.14	114.15	111.02
5	D	501	NAG	O5-C1-C2	2.15	114.47	111.47

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 [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	109/132 (82%)	-0.19	1 (0%) 84 66	17, 52, 107, 169	0
2	C	250/380 (65%)	0.04	7 (2%) 53 28	25, 59, 125, 204	0
3	B	108/132 (81%)	-0.20	0 100 100	20, 48, 93, 145	0
4	D	284/380 (74%)	-0.20	0 100 100	18, 44, 90, 143	1 (0%)
All	All	751/1024 (73%)	-0.12	8 (1%) 80 61	17, 51, 111, 204	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	262	LEU	3.6
2	C	167	THR	2.8
1	A	40	THR	2.6
2	C	217	SER	2.6
2	C	243	TYR	2.3
2	C	216	GLY	2.2
2	C	327	ASP	2.1
2	C	290	ASN	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

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
3	MLY	B	89	11/12	0.96	0.20	-	24,35,45,46	0
2	MLY	C	139	11/12	0.79	0.36	-	66,89,95,97	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MLY	D	99	11/12	0.94	0.24	-	33,35,47,51	0
2	MLY	C	104	11/12	0.97	0.22	-	29,33,54,64	0
4	MLY	D	82	11/12	0.96	0.27	-	33,36,40,40	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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( $\text{\AA}^2$ )	Q<0.9
5	NAG	D	501	14/15	0.82	0.22	0.37	78,80,83,84	0
5	NAG	C	501	14/15	0.84	0.27	0.22	67,69,71,72	0
6	CA	D	381	1/1	0.94	0.26	-	70,70,70,70	0
6	CA	C	381	1/1	0.97	0.19	-	85,85,85,85	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.