



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:24 PM GMT

PDB ID : 4LHU
Title : Crystal Structure of 9C2 TCR bound to CD1d
Authors : Uldrich, A.P.; Le Nours, J.; Pellicci, D.G.; Gras, S.; Rossjohn, J.; Godfrey, D.I.
Deposited on : 2013-07-01
Resolution : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

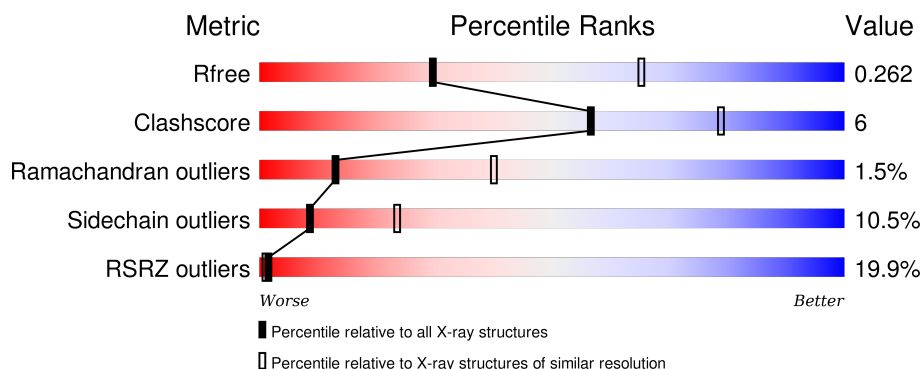
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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 ≥ 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	278	<div> <div>13%</div> <div>78%</div> <div>18%</div> <div>••</div> </div>
2	B	100	<div> <div>10%</div> <div>83%</div> <div>13%</div> <div>•</div> </div>
3	D	236	<div> <div>19%</div> <div>69%</div> <div>15%</div> <div>•</div> <div>14%</div> </div>
4	G	251	<div> <div>26%</div> <div>70%</div> <div>15%</div> <div>5%</div> <div>10%</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
11	CL	G	301	-	-	-	X
9	JLS	A	308	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6749 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2185	1397	382	399	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	HIS	-	EXPRESSION TAG	UNP P15813
A	279	HIS	-	EXPRESSION TAG	UNP P15813
A	280	HIS	-	EXPRESSION TAG	UNP P15813
A	281	HIS	-	EXPRESSION TAG	UNP P15813
A	282	HIS	-	EXPRESSION TAG	UNP P15813
A	283	HIS	-	EXPRESSION TAG	UNP P15813

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called 9C2 TCR delta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	202	Total	C	N	O	S	4	0	0
			1592	1015	269	301	7			

- Molecule 4 is a protein called 9C2 TCR gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	227	Total	C	N	O	S	4	0	0
			1847	1183	312	346	6			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

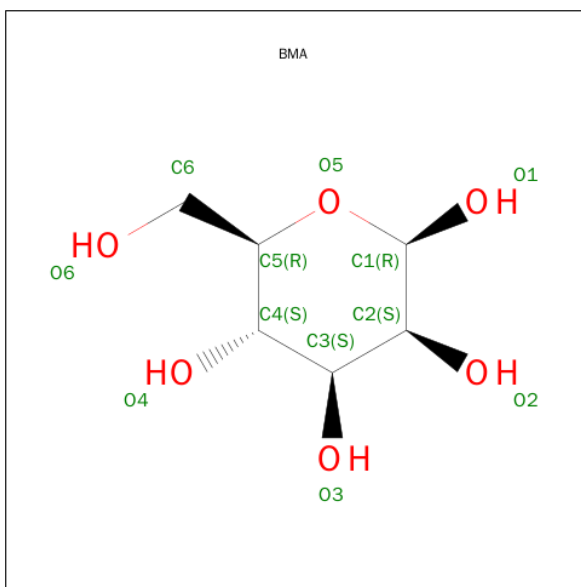


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

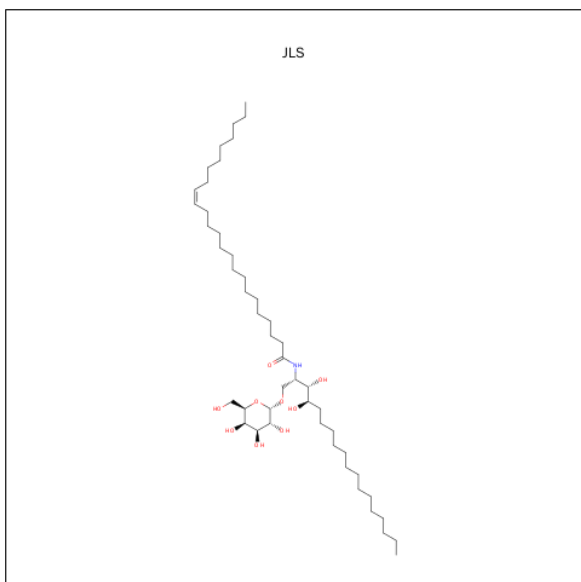


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is (15Z)-N-[(2S,3S,4R)-1-(ALPHA-D-GALACTOPYRANOSYLOXY)-3,4-DIHYDROXYOCTADECAN-2-YL]TETRACOS-15-ENAMIDE (three-letter code: JLS) (formula: C₄₈H₉₃NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			58	48	1	9		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	G	1	Total	Cl	0	0
			1	1		

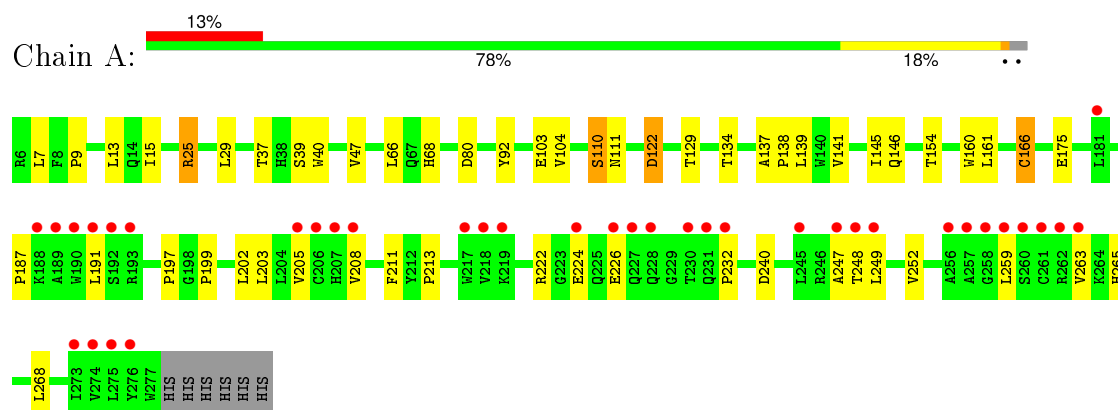
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	44	Total	O	0	0
			44	44		
12	B	6	Total	O	0	0
			6	6		
12	D	18	Total	O	0	0
			18	18		
12	G	41	Total	O	0	0
			41	41		

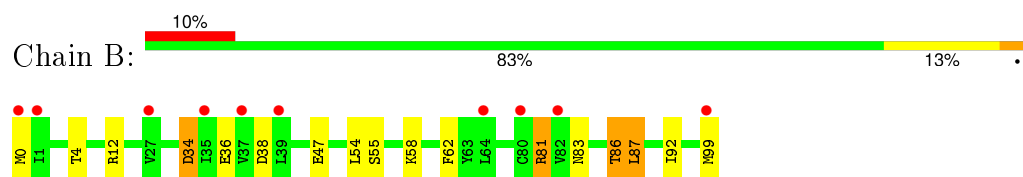
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

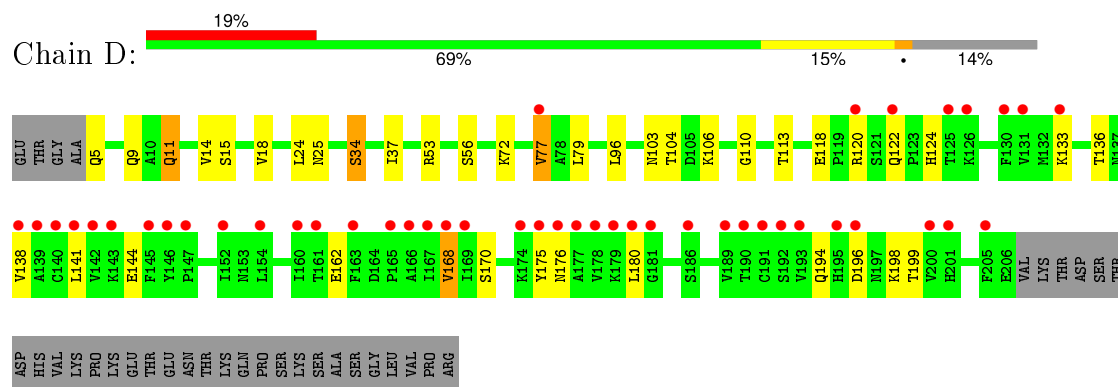
- Molecule 1: Antigen-presenting glycoprotein CD1d



- Molecule 2: Beta-2-microglobulin

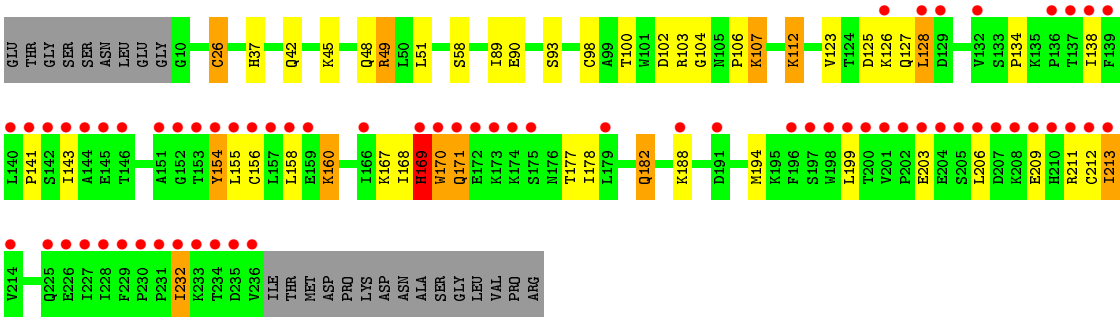


- Molecule 3: 9C2 TCR delta chain



- Molecule 4: 9C2 TCR gamma chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.62Å 152.69Å 135.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.47 – 2.87 47.47 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.47-2.87) 99.1 (47.47-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.206 , 0.243 0.223 , 0.262	Depositor DCC
R_{free} test set	1579 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31199 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, BMA, NAG, JLS, CL

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	0.43	0/2250	0.64	0/3063
2	B	0.40	0/859	0.61	0/1162
3	D	0.44	0/1627	0.64	0/2200
4	G	0.47	0/1896	0.65	1/2576 (0.0%)
All	All	0.44	0/6632	0.64	1/9001 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	103	ARG	C-N-CA	5.80	134.47	122.30

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	2185	0	2121	22	0
2	B	836	0	805	8	0
3	D	1592	0	1600	14	0
4	G	1847	0	1830	43	0
5	A	14	0	13	0	0
6	A	56	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	11	0	10	0	0
8	A	1	0	0	0	0
9	A	58	0	93	3	0
10	D	39	0	34	1	0
11	G	1	0	0	0	0
12	A	44	0	0	0	0
12	B	6	0	0	0	0
12	D	18	0	0	0	0
12	G	41	0	0	0	0
All	All	6749	0	6556	78	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 6.

All (78) 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:G:170:TRP:CZ2	4:G:212:CYS:HB2	1.96	0.99
4:G:26:CYS:HG	4:G:98:CYS:HG	1.21	0.85
4:G:169:HIS:O	4:G:170:TRP:HB2	1.75	0.84
4:G:169:HIS:O	4:G:170:TRP:CB	2.30	0.79
4:G:170:TRP:CZ2	4:G:212:CYS:CB	2.65	0.79
4:G:170:TRP:CE2	4:G:212:CYS:HA	2.21	0.75
4:G:169:HIS:O	4:G:170:TRP:CD1	2.44	0.70
3:D:11:GLN:O	3:D:113:THR:HG22	1.93	0.68
1:A:122:ASP:HB3	1:A:134:THR:HG21	1.83	0.60
4:G:169:HIS:O	4:G:170:TRP:CG	2.55	0.59
4:G:171:GLN:HA	4:G:177:THR:O	2.03	0.59
3:D:9:GLN:HE21	3:D:110:GLY:HA3	1.68	0.59
1:A:205:VAL:HG21	2:B:99:MET:HG2	1.87	0.57
4:G:170:TRP:CZ2	4:G:212:CYS:SG	2.98	0.57
4:G:93:SER:HB3	4:G:123:VAL:HG22	1.88	0.56
4:G:134:PRO:HB2	4:G:158:LEU:HD22	1.89	0.55
4:G:169:HIS:HB2	4:G:213:ILE:CD1	2.37	0.55
4:G:170:TRP:NE1	4:G:212:CYS:HA	2.22	0.53
1:A:154:THR:HG21	9:A:308:JLS:H61	1.91	0.53
4:G:167:LYS:O	4:G:168:ILE:CG2	2.57	0.53
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.90	0.53
1:A:9:PRO:HB3	1:A:103:GLU:HB3	1.92	0.52
2:B:4:THR:HA	2:B:86:THR:HG21	1.91	0.52
4:G:170:TRP:CE2	4:G:212:CYS:CB	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:37:ILE:HG21	3:D:77:VAL:HG21	1.93	0.51
1:A:104:VAL:HG12	1:A:110:SER:HB2	1.91	0.51
3:D:175:TYR:HE2	4:G:182:GLN:HG2	1.75	0.51
4:G:167:LYS:O	4:G:168:ILE:HG23	2.11	0.51
4:G:170:TRP:C	4:G:171:GLN:HG2	2.31	0.50
1:A:232:PRO:HA	1:A:247:ALA:HA	1.94	0.50
1:A:68:HIS:HE1	3:D:103:ASN:OD1	1.95	0.50
4:G:37:HIS:HD2	4:G:49:ARG:HE	1.58	0.50
2:B:81:ARG:HB3	2:B:92:ILE:HG22	1.94	0.49
4:G:170:TRP:CE2	4:G:212:CYS:CA	2.95	0.49
3:D:194:GLN:HA	3:D:199:THR:HA	1.95	0.49
3:D:104:THR:O	4:G:49:ARG:NH2	2.47	0.48
4:G:167:LYS:C	4:G:168:ILE:HG23	2.34	0.48
1:A:213:PRO:HD2	1:A:265:HIS:HE1	1.78	0.47
1:A:208:VAL:HG21	1:A:263:VAL:HG11	1.96	0.47
4:G:154:TYR:HE2	4:G:199:LEU:HD23	1.79	0.47
4:G:206:LEU:HD22	4:G:232:ILE:HB	1.97	0.47
1:A:160:TRP:CD1	3:D:34:SER:HB3	2.50	0.47
2:B:36:GLU:HB2	2:B:83:ASN:HB3	1.96	0.47
1:A:80:ASP:OD2	9:A:308:JLS:H57	2.15	0.47
4:G:203:GLU:HA	4:G:206:LEU:HD12	1.96	0.46
1:A:141:VAL:O	1:A:145:ILE:HG12	2.16	0.46
4:G:89:ILE:O	4:G:123:VAL:HG21	2.15	0.46
1:A:25:ARG:HB2	6:A:304:NAG:H82	1.98	0.46
1:A:213:PRO:HD2	1:A:265:HIS:CE1	2.51	0.45
4:G:170:TRP:NE1	4:G:212:CYS:SG	2.90	0.45
3:D:175:TYR:CE2	4:G:182:GLN:HG2	2.52	0.44
4:G:168:ILE:C	4:G:169:HIS:CG	2.90	0.44
4:G:169:HIS:HB2	4:G:170:TRP:H	1.52	0.44
1:A:161:LEU:O	1:A:166:CYS:HB2	2.17	0.44
4:G:102:ASP:OD2	4:G:104:GLY:HA2	2.17	0.44
4:G:104:GLY:HA3	4:G:112:LYS:HE2	2.00	0.44
4:G:141:PRO:HB2	4:G:232:ILE:HG12	1.99	0.44
1:A:240:ASP:HB2	2:B:12:ARG:HE	1.83	0.44
3:D:170:SER:HB3	3:D:175:TYR:HA	1.99	0.44
4:G:42:GLN:HB2	4:G:45:LYS:HD2	2.00	0.43
4:G:170:TRP:HZ2	4:G:212:CYS:SG	2.40	0.43
1:A:205:VAL:HG22	1:A:248:THR:HG22	2.01	0.43
10:D:401:NAG:H4	4:G:138:ILE:HD11	2.01	0.43
3:D:24:LEU:HD12	3:D:79:LEU:HD23	2.00	0.43
4:G:160:LYS:H	4:G:160:LYS:HZ2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PRO:HG3	1:A:203:LEU:HD23	2.01	0.42
4:G:126:LYS:HB3	4:G:128:LEU:HD12	2.00	0.42
3:D:106:LYS:HB3	4:G:49:ARG:CZ	2.49	0.42
3:D:18:VAL:HG23	3:D:118:GLU:O	2.19	0.42
3:D:133:LYS:HB3	3:D:138:VAL:HG23	2.02	0.42
4:G:143:ILE:HG13	4:G:143:ILE:H	1.75	0.42
4:G:106:PRO:HD2	4:G:112:LYS:NZ	2.35	0.42
2:B:83:ASN:HA	2:B:87:LEU:HD11	2.00	0.41
1:A:29:LEU:HD11	2:B:55:SER:HB2	2.01	0.41
1:A:47:VAL:HG11	9:A:308:JLS:H29	2.03	0.41
4:G:104:GLY:H	4:G:107:LYS:HA	1.86	0.41
1:A:137:ALA:C	1:A:139:LEU:H	2.24	0.41
1:A:187:PRO:HB3	1:A:211:PHE:HB3	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	270/278 (97%)	250 (93%)	17 (6%)	3 (1%)	17	49
2	B	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	19	52
3	D	200/236 (85%)	181 (90%)	15 (8%)	4 (2%)	9	32
4	G	225/251 (90%)	204 (91%)	17 (8%)	4 (2%)	11	35
All	All	793/865 (92%)	730 (92%)	51 (6%)	12 (2%)	13	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PRO
4	G	170	TRP

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Mol	Chain	Res	Type
2	B	34	ASP
3	D	124	HIS
3	D	144	GLU
3	D	196	ASP
4	G	125	ASP
4	G	169	HIS
4	G	107	LYS
3	D	168	VAL
1	A	138	PRO
1	A	252	VAL

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	238/244 (98%)	214 (90%)	24 (10%)	9	26
2	B	95/95 (100%)	87 (92%)	8 (8%)	14	36
3	D	180/210 (86%)	160 (89%)	20 (11%)	8	20
4	G	208/228 (91%)	184 (88%)	24 (12%)	7	19
All	All	721/777 (93%)	645 (90%)	76 (10%)	8	23

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	13	LEU
1	A	15	ILE
1	A	25	ARG
1	A	37	THR
1	A	39	SER
1	A	40	TRP
1	A	66	LEU
1	A	92	TYR
1	A	110	SER
1	A	111	ASN

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Mol	Chain	Res	Type
1	A	122	ASP
1	A	129	THR
1	A	146	GLN
1	A	166	CYS
1	A	175	GLU
1	A	191	LEU
1	A	202	LEU
1	A	222	ARG
1	A	224	GLU
1	A	226	GLU
1	A	249	LEU
1	A	259	LEU
1	A	268	LEU
2	B	0	MET
2	B	34	ASP
2	B	38	ASP
2	B	47	GLU
2	B	58	LYS
2	B	81	ARG
2	B	86	THR
2	B	87	LEU
3	D	5	GLN
3	D	11	GLN
3	D	14	VAL
3	D	15	SER
3	D	25	ASN
3	D	34	SER
3	D	53	ARG
3	D	56	SER
3	D	72	LYS
3	D	77	VAL
3	D	96	LEU
3	D	120	ARG
3	D	122	GLN
3	D	136	THR
3	D	141	LEU
3	D	162	GLU
3	D	168	VAL
3	D	176	ASN
3	D	180	LEU
3	D	198	LYS
4	G	26	CYS

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Mol	Chain	Res	Type
4	G	48	GLN
4	G	49	ARG
4	G	51	LEU
4	G	58	SER
4	G	90	GLU
4	G	100	THR
4	G	112	LYS
4	G	127	GLN
4	G	128	LEU
4	G	154	TYR
4	G	155	LEU
4	G	156	CYS
4	G	160	LYS
4	G	169	HIS
4	G	171	GLN
4	G	178	ILE
4	G	182	GLN
4	G	188	LYS
4	G	194	MET
4	G	209	GLU
4	G	211	ARG
4	G	213	ILE
4	G	232	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	184	GLN
1	A	238	ASN
3	D	9	GLN
3	D	60	ASN
3	D	85	GLN
3	D	122	GLN
4	G	37	HIS
4	G	48	GLN
4	G	169	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 ⓘ

7 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
6	NAG	A	302	1,6	14,14,15	1.89	2 (14%)	15,19,21	2.05	4 (26%)
6	NAG	A	303	6	14,14,15	1.77	3 (21%)	15,19,21	1.68	3 (20%)
6	NAG	A	304	1,6	14,14,15	1.83	5 (35%)	15,19,21	1.62	3 (20%)
6	NAG	A	305	6	14,14,15	1.82	3 (21%)	15,19,21	1.42	2 (13%)
10	NAG	D	401	10,3	14,14,15	1.80	3 (21%)	15,19,21	2.17	5 (33%)
10	NAG	D	402	10	14,14,15	1.81	2 (14%)	15,19,21	1.98	5 (33%)
10	BMA	D	403	10	11,11,12	1.87	3 (27%)	14,15,17	1.50	2 (14%)

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
6	NAG	A	302	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	303	6	-	0/6/23/26	0/1/1/1
6	NAG	A	304	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	305	6	-	0/6/23/26	0/1/1/1
10	NAG	D	401	10,3	-	0/6/23/26	0/1/1/1
10	NAG	D	402	10	-	0/6/23/26	0/1/1/1
10	BMA	D	403	10	-	0/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	403	BMA	C4-C3	-4.51	1.40	1.52
6	A	304	NAG	C1-C2	-2.94	1.48	1.52
10	D	403	BMA	C2-C3	-2.80	1.48	1.52
6	A	304	NAG	C3-C2	-2.34	1.46	1.52
10	D	403	BMA	O5-C1	-2.20	1.40	1.43
6	A	304	NAG	C4-C3	-2.17	1.46	1.52
6	A	303	NAG	C4-C3	-2.06	1.47	1.52
10	D	401	NAG	C4-C3	-2.05	1.47	1.52
6	A	305	NAG	C4-C3	-2.01	1.47	1.52
6	A	304	NAG	C7-N2	2.43	1.43	1.34
6	A	303	NAG	C7-N2	2.75	1.44	1.34
10	D	401	NAG	C7-N2	2.83	1.45	1.34
6	A	305	NAG	C7-N2	2.88	1.45	1.34
10	D	402	NAG	C7-N2	2.89	1.45	1.34
6	A	302	NAG	C7-N2	2.90	1.45	1.34
6	A	304	NAG	O5-C1	3.89	1.50	1.43
6	A	303	NAG	O5-C1	4.26	1.50	1.43
10	D	401	NAG	O5-C1	4.47	1.51	1.43
10	D	402	NAG	O5-C1	4.59	1.51	1.43
6	A	305	NAG	O5-C1	4.67	1.51	1.43
6	A	302	NAG	O5-C1	4.80	1.51	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	403	BMA	O4-C4-C3	-2.23	105.32	110.34
10	D	401	NAG	O4-C4-C3	-2.13	105.53	110.34
6	A	304	NAG	O3-C3-C2	-2.03	105.09	109.11
6	A	304	NAG	O5-C5-C6	2.01	111.70	107.35
10	D	402	NAG	O5-C5-C6	2.06	111.80	107.35
6	A	302	NAG	O6-C6-C5	2.20	118.61	111.33
6	A	305	NAG	C1-O5-C5	2.27	115.13	112.25
10	D	401	NAG	O6-C6-C5	2.28	118.88	111.33
10	D	402	NAG	O4-C4-C5	2.31	115.35	109.24
6	A	303	NAG	C3-C4-C5	2.44	114.45	110.20
6	A	303	NAG	O5-C5-C6	2.49	112.74	107.35
10	D	401	NAG	C3-C4-C5	2.51	114.57	110.20
10	D	403	BMA	C2-C3-C4	3.05	116.22	111.04
6	A	302	NAG	C4-C3-C2	3.23	116.25	111.23
6	A	305	NAG	O5-C5-C6	3.42	114.75	107.35
10	D	402	NAG	C1-O5-C5	3.43	116.60	112.25
10	D	402	NAG	C4-C3-C2	3.44	116.58	111.23
6	A	302	NAG	O5-C5-C6	3.58	115.09	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	401	NAG	O5-C5-C6	3.65	115.25	107.35
10	D	402	NAG	C3-C4-C5	3.70	116.65	110.20
6	A	303	NAG	C4-C3-C2	4.03	117.50	111.23
6	A	304	NAG	C1-O5-C5	4.39	117.82	112.25
6	A	302	NAG	C1-O5-C5	4.76	118.28	112.25
10	D	401	NAG	C4-C3-C2	5.72	120.12	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	304	NAG	1	0
10	D	401	NAG	1	0

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	A	301	1	14,14,15	1.90	3 (21%)	15,19,21	1.73	5 (33%)
7	BMA	A	306	-	11,11,12	1.88	3 (27%)	14,15,17	2.21	6 (42%)
9	JLS	A	308	-	57,58,58	0.41	0	63,67,67	1.03	7 (11%)

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	A	301	1	-	0/6/23/26	0/1/1/1
7	BMA	A	306	-	-	0/2/19/22	0/1/1/1
9	JLS	A	308	-	-	0/56/76/76	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	306	BMA	C4-C3	-4.54	1.40	1.52
7	A	306	BMA	C2-C3	-2.75	1.48	1.52
5	A	301	NAG	C4-C3	-2.18	1.46	1.52
7	A	306	BMA	O5-C1	-2.14	1.40	1.43
5	A	301	NAG	C7-N2	2.70	1.44	1.34
5	A	301	NAG	O5-C1	5.20	1.52	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	308	JLS	CAC-CAB-CAA	-2.96	105.40	113.24
7	A	306	BMA	O4-C4-C3	-2.75	104.14	110.34
9	A	308	JLS	OAA-CAA-CAB	-2.37	117.89	121.98
9	A	308	JLS	C6-C5-C4	-2.06	110.51	114.20
9	A	308	JLS	O1A-C1A-C2A	2.02	110.59	108.04
5	A	301	NAG	C3-C4-C5	2.09	113.84	110.20
9	A	308	JLS	C1A-O5A-C5M	2.13	117.88	113.75
9	A	308	JLS	O4-C4-C3	2.15	114.43	109.02
9	A	308	JLS	O5A-C5M-C6A	2.21	111.93	106.36
5	A	301	NAG	C4-C3-C2	2.21	114.66	111.23
5	A	301	NAG	O6-C6-C5	2.25	118.78	111.33
7	A	306	BMA	O6-C6-C5	2.26	118.79	111.33
5	A	301	NAG	C1-O5-C5	2.57	115.50	112.25
7	A	306	BMA	C1-O5-C5	2.85	115.86	112.25
7	A	306	BMA	C1-C2-C3	3.07	113.17	109.54
7	A	306	BMA	C3-C4-C5	3.13	115.65	110.20
5	A	301	NAG	O5-C5-C6	4.03	116.08	107.35
7	A	306	BMA	C2-C3-C4	4.55	118.76	111.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	308	JLS	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	272/278 (97%)	0.72	37 (13%)	4 2	45, 88, 201, 212	0
2	B	100/100 (100%)	0.64	10 (10%)	9 5	74, 118, 154, 199	0
3	D	202/236 (85%)	1.39	46 (22%)	1 1	48, 109, 226, 240	2 (0%)
4	G	227/251 (90%)	1.78	66 (29%)	1 0	45, 105, 209, 227	1 (0%)
All	All	801/865 (92%)	1.18	159 (19%)	1 1	45, 104, 209, 240	3 (0%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	180	LEU	15.4
3	D	177	ALA	15.2
4	G	228	ILE	11.5
3	D	165	PRO	11.4
3	D	178	VAL	11.0
4	G	230	PRO	10.1
4	G	227	ILE	9.7
3	D	192	SER	9.7
4	G	153	THR	9.2
4	G	234	THR	9.0
3	D	191	CYS	8.9
4	G	235	ASP	8.7
4	G	154	TYR	8.7
3	D	142	VAL	8.6
4	G	175	SER	8.6
4	G	152	GLY	8.4
3	D	179	LYS	8.3
3	D	167	ILE	8.2
4	G	174	LYS	8.1
3	D	166	ALA	8.0
4	G	140	LEU	7.5

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Mol	Chain	Res	Type	RSRZ
4	G	128	LEU	7.5
4	G	199	LEU	7.4
4	G	139	PHE	7.2
4	G	229	PHE	7.1
4	G	138	ILE	6.9
4	G	209	GLU	6.8
4	G	197	SER	6.8
4	G	142	SER	6.7
4	G	236	VAL	6.5
4	G	231	PRO	6.4
4	G	157	LEU	6.3
3	D	196	ASP	6.2
1	A	208	VAL	6.1
4	G	233	LYS	6.1
4	G	208	LYS	5.9
3	D	141	LEU	5.9
1	A	206	CYS	5.7
4	G	211	ARG	5.6
4	G	137	THR	5.5
4	G	232	ILE	5.4
3	D	154	LEU	5.4
4	G	207	ASP	5.4
4	G	145	GLU	5.3
3	D	193	VAL	5.3
2	B	99	MET	5.3
4	G	141	PRO	5.3
1	A	261	CYS	5.2
1	A	191	LEU	5.2
2	B	39	LEU	5.2
4	G	210	HIS	5.1
4	G	200	THR	4.9
4	G	126	LYS	4.9
4	G	196	PHE	4.9
1	A	256	ALA	4.7
3	D	168	VAL	4.7
4	G	151	ALA	4.6
3	D	201	HIS	4.6
4	G	156	CYS	4.6
3	D	190	THR	4.6
4	G	143	ILE	4.5
4	G	212	CYS	4.4
1	A	189	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	205	VAL	4.3
1	A	245	LEU	4.3
3	D	140	CYS	4.2
2	B	37	VAL	4.2
3	D	195	HIS	4.2
4	G	144	ALA	4.1
1	A	218	VAL	4.0
4	G	172	GLU	4.0
4	G	226	GLU	3.9
1	A	231	GLN	3.9
3	D	122	GLN	3.9
1	A	263	VAL	3.9
3	D	126	LYS	3.9
4	G	214	VAL	3.9
4	G	170	TRP	3.8
4	G	158	LEU	3.8
4	G	179	LEU	3.7
1	A	247	ALA	3.7
1	A	228	GLN	3.7
3	D	200	VAL	3.6
4	G	201	VAL	3.6
4	G	169	HIS	3.6
4	G	155	LEU	3.5
4	G	203	GLU	3.5
2	B	80	CYS	3.5
3	D	139	ALA	3.5
1	A	219	LYS	3.4
1	A	207	HIS	3.4
1	A	259	LEU	3.4
3	D	143	LYS	3.3
4	G	159	GLU	3.3
2	B	35	ILE	3.2
3	D	161	THR	3.2
3	D	163	PHE	3.2
4	G	136	PRO	3.2
4	G	206	LEU	3.2
1	A	249	LEU	3.1
3	D	146	TYR	3.0
1	A	217	TRP	3.0
3	D	138	VAL	3.0
3	D	120	ARG	3.0
3	D	176	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
4	G	202	PRO	3.0
1	A	260	SER	3.0
1	A	273	ILE	2.9
3	D	131	VAL	2.9
3	D	205	PHE	2.9
4	G	171	GLN	2.9
2	B	0	MET	2.9
1	A	248	THR	2.9
4	G	204	GLU	2.8
4	G	166	ILE	2.8
4	G	188	LYS	2.8
4	G	225	GLN	2.8
3	D	130	PHE	2.7
3	D	181	GLY	2.7
2	B	64	LEU	2.7
1	A	257	ALA	2.7
4	G	205	SER	2.7
3	D	175	TYR	2.6
3	D	147	PRO	2.6
1	A	190	TRP	2.6
2	B	27	VAL	2.6
1	A	274	VAL	2.6
1	A	193	ARG	2.6
3	D	133	LYS	2.5
3	D	174	LYS	2.5
4	G	132	VAL	2.5
3	D	145	PHE	2.5
4	G	173	LYS	2.4
1	A	262	ARG	2.4
4	G	213	ILE	2.4
3	D	77	VAL	2.4
3	D	160	ILE	2.4
3	D	169	ILE	2.4
4	G	198	TRP	2.4
2	B	82	VAL	2.3
3	D	186	SER	2.3
3	D	125	THR	2.3
1	A	192	SER	2.2
3	D	189	VAL	2.2
4	G	129	ASP	2.2
1	A	181	LEU	2.2
1	A	188	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	THR	2.2
1	A	275	LEU	2.2
3	D	152	ILE	2.2
1	A	258	GLY	2.2
1	A	276	TYR	2.2
4	G	146	THR	2.1
1	A	226	GLU	2.1
1	A	227	GLN	2.1
1	A	224	GLU	2.1
2	B	1	ILE	2.1
4	G	191	ASP	2.1
1	A	232	PRO	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	A	302	14/15	0.92	0.13	-	110,115,121,124	0
10	NAG	D	401	14/15	0.86	0.17	-	185,195,200,200	0
6	NAG	A	304	14/15	0.96	0.19	-	73,81,86,94	0
6	NAG	A	303	14/15	0.91	0.17	-	117,130,135,136	0
10	BMA	D	403	11/12	0.84	0.18	-	185,198,203,204	0
6	NAG	A	305	14/15	0.91	0.14	-	105,111,118,121	0
10	NAG	D	402	14/15	0.87	0.22	-	193,201,205,207	0

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, 95th 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(\AA^2)	Q<0.9
9	JLS	A	308	58/58	0.94	0.45	4.99	47,63,84,85	0
11	CL	G	301	1/1	0.98	0.34	4.36	70,70,70,70	0
8	MG	A	307	1/1	0.83	0.35	-	80,80,80,80	0
7	BMA	A	306	11/12	0.60	0.17	-	176,178,181,182	0
5	NAG	A	301	14/15	0.74	0.24	-	124,129,134,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.