



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:26 AM GMT

PDB ID : 3AU1
Title : Crystal structure of mouse CD1d in complex with ganglioside GD3
Authors : Roisman, L.C.; Rossjohn, J.
Deposited on : 2011-01-28
Resolution : 2.50 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

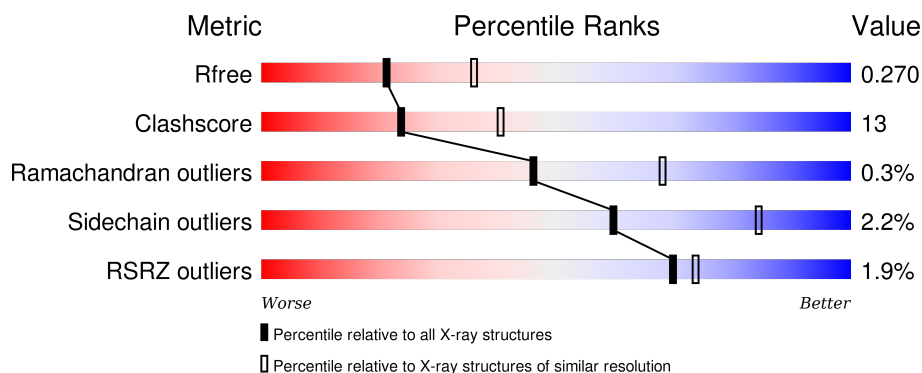
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	302	<div> <div>2%</div> <div>64%</div> <div>24%</div> <div>12%</div> </div>
2	B	99	<div> <div>%</div> <div>76%</div> <div>20%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	307	X	-	-	X
4	MAN	A	308	X	-	-	-
5	GLC	A	311	X	-	-	-
5	BMA	A	312	-	-	-	X
6	ERA	A	315	X	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3197 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 CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2115	1355	359	388	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	EXPRESSION TAG	UNP P11609
A	282	LEU	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	ILE	-	EXPRESSION TAG	UNP P11609
A	286	LEU	-	EXPRESSION TAG	UNP P11609
A	287	ASP	-	EXPRESSION TAG	UNP P11609
A	288	ALA	-	EXPRESSION TAG	UNP P11609
A	289	GLN	-	EXPRESSION TAG	UNP P11609
A	290	LYS	-	EXPRESSION TAG	UNP P11609
A	291	MET	-	EXPRESSION TAG	UNP P11609
A	292	VAL	-	EXPRESSION TAG	UNP P11609
A	293	TRP	-	EXPRESSION TAG	UNP P11609
A	294	ASN	-	EXPRESSION TAG	UNP P11609
A	295	HIS	-	EXPRESSION TAG	UNP P11609
A	296	ARG	-	EXPRESSION TAG	UNP P11609
A	297	HIS	-	EXPRESSION TAG	UNP P11609
A	298	HIS	-	EXPRESSION TAG	UNP P11609
A	299	HIS	-	EXPRESSION TAG	UNP P11609
A	300	HIS	-	EXPRESSION TAG	UNP P11609
A	301	HIS	-	EXPRESSION TAG	UNP P11609
A	302	HIS	-	EXPRESSION TAG	UNP P11609

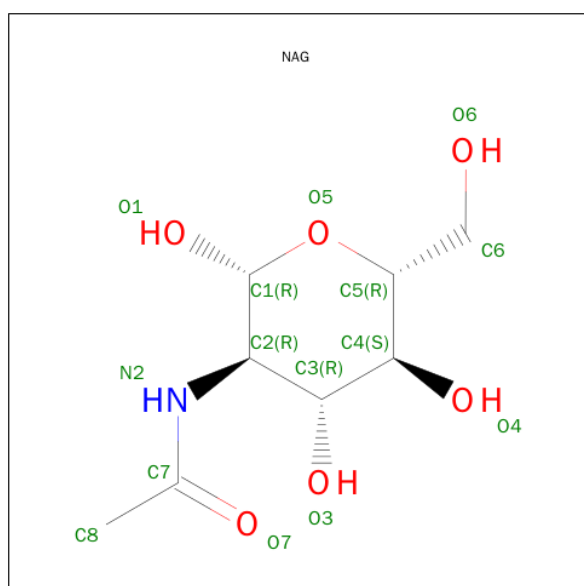
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			796	508	132	149	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

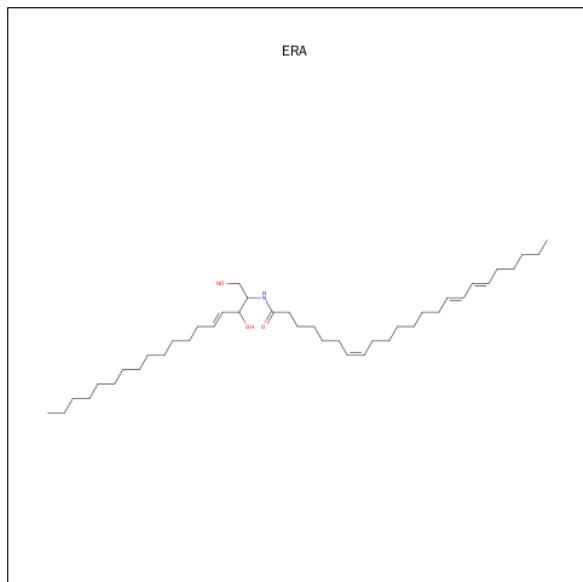
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 6 is (7Z,15E,17E)-N-[(2S,3S,4E)-1,3-DIHYDROXYOCTADEC-4-EN-2-YL]TRIC OSA-7,15,17-TRIENAMIDE (three-letter code: ERA) (formula: $C_{41}H_{75}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			41	37	1	3		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	2	Total	C	O	0	0
			22	12	10		

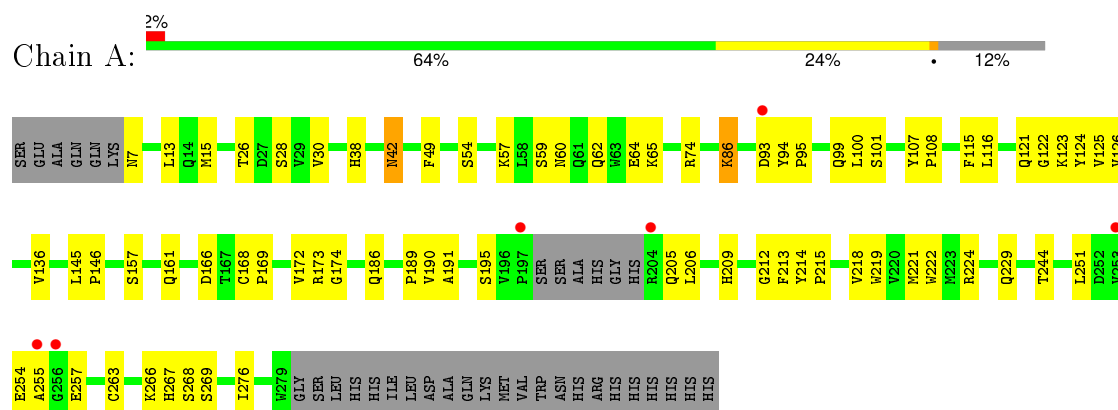
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	0
			49	49		
8	B	28	Total	O	0	0
			28	28		

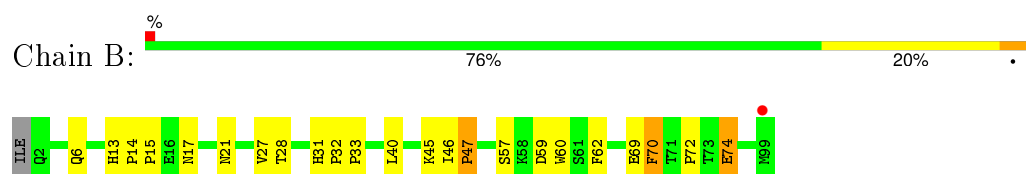
3 Residue-property plots [i](#)

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 CD1d1



- Molecule 2: Beta-2-microglobulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.66Å 98.45Å 55.49Å 90.00° 106.68° 90.00°	Depositor
Resolution (Å)	49.21 – 2.50 49.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.21-2.50) 98.4 (49.22-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.194 , 0.238 0.226 , 0.270	Depositor DCC
R_{free} test set	735 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 14670 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3197	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NAG, GLC, FUC, GAL, BMA, MAN, ERA

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	0/2177	0.55	0/2964
2	B	0.43	0/822	0.56	0/1118
All	All	0.43	0/2999	0.55	0/4082

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
4	A	2	0
5	A	1	0
All	All	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	307	MAN	C1
4	A	308	MAN	C1
5	A	311	GLC	C1

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2115	0	2006	62	0
2	B	796	0	750	16	0
3	A	14	0	13	0	0
4	A	61	0	52	2	0
5	A	71	0	61	1	0
6	A	41	0	57	0	0
7	A	22	0	19	0	0
8	A	49	0	0	5	0
8	B	28	0	0	5	0
All	All	3197	0	2958	80	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 13.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:O	1:A:64:GLU:HG2	1.70	0.91
2:B:15:PRO:HA	8:B:114:HOH:O	1.81	0.79
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.69	0.73
1:A:267:HIS:HD2	1:A:269:SER:OG	1.72	0.72
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.72	0.71
2:B:74:GLU:HA	2:B:74:GLU:OE1	1.90	0.69
1:A:166:ASP:O	1:A:169:PRO:HD2	1.92	0.69
1:A:190:VAL:HG21	8:B:124:HOH:O	1.91	0.69
2:B:17:ASN:HA	2:B:72:PRO:O	1.94	0.67
1:A:62:GLN:HA	1:A:65:LYS:HE2	1.79	0.63
1:A:122:GLY:N	8:A:318:HOH:O	2.30	0.62
1:A:205:GLN:HB3	8:A:348:HOH:O	2.00	0.62
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.82	0.62
1:A:191:ALA:HA	1:A:209:HIS:O	2.00	0.61
1:A:267:HIS:CD2	1:A:269:SER:H	2.18	0.61
1:A:254:GLU:O	1:A:257:GLU:HB3	2.00	0.61
1:A:59:SER:OG	1:A:62:GLN:HG3	2.01	0.61
1:A:224:ARG:HB2	1:A:229:GLN:HE21	1.65	0.60
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.86	0.57
1:A:267:HIS:CD2	1:A:269:SER:OG	2.56	0.57
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.87	0.56
1:A:59:SER:HB3	1:A:62:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:HA	1:A:229:GLN:OE1	2.06	0.55
1:A:62:GLN:HA	1:A:65:LYS:CE	2.36	0.55
1:A:276:ILE:N	1:A:276:ILE:HD12	2.22	0.55
1:A:168:CYS:O	1:A:172:VAL:HG23	2.08	0.54
1:A:215:PRO:O	1:A:267:HIS:HE1	1.92	0.53
5:A:311:GLC:O2	5:A:313:MAN:H5	2.10	0.52
1:A:59:SER:H	1:A:62:GLN:NE2	2.07	0.52
1:A:195:SER:HB3	1:A:206:LEU:HD23	1.92	0.52
1:A:218:VAL:HG22	1:A:219:TRP:N	2.24	0.52
2:B:57:SER:HB2	2:B:59:ASP:OD1	2.09	0.52
1:A:224:ARG:HB2	1:A:229:GLN:NE2	2.25	0.51
1:A:125:VAL:HG23	1:A:126:VAL:HG23	1.93	0.51
1:A:255:ALA:C	1:A:257:GLU:H	2.12	0.51
1:A:189:PRO:HB3	1:A:213:PHE:HB3	1.92	0.51
1:A:219:TRP:CH2	1:A:221:MET:HB3	2.47	0.50
1:A:123:LYS:HE3	8:B:126:HOH:O	2.10	0.50
1:A:7:ASN:OD1	1:A:108:PRO:HD3	2.12	0.50
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.93	0.49
2:B:28:THR:HG23	8:B:113:HOH:O	2.11	0.49
1:A:100:LEU:HD23	1:A:101:SER:N	2.28	0.49
4:A:307:MAN:C1	4:A:308:MAN:H5	2.43	0.49
1:A:219:TRP:CE3	1:A:266:LYS:HG3	2.47	0.49
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.78	0.48
1:A:74:ARG:HD2	8:A:322:HOH:O	2.14	0.48
1:A:30:VAL:CG2	1:A:38:HIS:HB2	2.44	0.47
2:B:31:HIS:ND1	8:B:100:HOH:O	2.36	0.47
1:A:145:LEU:HB3	1:A:146:PRO:CD	2.43	0.47
1:A:214:TYR:CG	1:A:215:PRO:HA	2.49	0.47
1:A:49:PHE:HB3	1:A:54:SER:HB2	1.95	0.47
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.97	0.46
1:A:222:TRP:CB	1:A:251:LEU:HD22	2.45	0.46
2:B:6:GLN:O	2:B:27:VAL:HA	2.15	0.46
1:A:57:LYS:HG3	1:A:174:GLY:HA2	1.98	0.46
2:B:59:ASP:O	2:B:60:TRP:HB2	2.16	0.45
1:A:263:CYS:O	1:A:276:ILE:HA	2.15	0.45
1:A:100:LEU:HD23	1:A:100:LEU:C	2.36	0.45
4:A:306:GLC:O2	4:A:307:MAN:H5	2.17	0.45
1:A:94:TYR:HB3	1:A:95:PRO:HA	1.99	0.45
1:A:13:LEU:O	1:A:28:SER:HA	2.16	0.45
1:A:121:GLN:HA	1:A:121:GLN:OE1	2.16	0.45
1:A:186:GLN:OE1	1:A:268:SER:OG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HD2	1:A:174:GLY:HA2	1.99	0.44
2:B:46:ILE:HA	2:B:47:PRO:HD3	1.76	0.44
1:A:212:GLY:HA2	1:A:244:THR:OG1	2.18	0.43
1:A:116:LEU:C	1:A:116:LEU:HD23	2.39	0.43
1:A:115:PHE:HA	8:A:320:HOH:O	2.19	0.42
1:A:86:LYS:HB2	1:A:86:LYS:HE3	1.90	0.42
1:A:59:SER:H	1:A:62:GLN:HE21	1.65	0.42
2:B:33:PRO:HD3	2:B:62:PHE:CE1	2.54	0.42
1:A:26:THR:O	1:A:42:ASN:HB2	2.19	0.42
1:A:214:TYR:CD1	1:A:215:PRO:HA	2.55	0.42
2:B:21:ASN:HB3	2:B:70:PHE:CE2	2.55	0.41
1:A:62:GLN:O	1:A:65:LYS:HB2	2.20	0.41
1:A:123:LYS:HD3	1:A:123:LYS:HA	1.79	0.41
2:B:32:PRO:CB	2:B:33:PRO:HD2	2.47	0.41
1:A:99:GLN:HG3	8:A:332:HOH:O	2.21	0.41
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.56	0.41
1:A:157:SER:O	1:A:161:GLN:HG3	2.21	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	263/302 (87%)	255 (97%)	8 (3%)	0	100	100
2	B	96/99 (97%)	93 (97%)	2 (2%)	1 (1%)	19	34
All	All	359/401 (90%)	348 (97%)	10 (3%)	1 (0%)	46	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	47	PRO

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	226/264 (86%)	222 (98%)	4 (2%)	66	88
2	B	89/93 (96%)	86 (97%)	3 (3%)	44	72
All	All	315/357 (88%)	308 (98%)	7 (2%)	60	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	86	LYS
1	A	93	ASP
1	A	173	ARG
2	B	69	GLU
2	B	70	PHE
2	B	74	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	99	GLN
1	A	267	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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$
4	NAG	A	304	1,4	14,14,15	0.57	0	15,19,21	1.25	0
4	NAG	A	305	4	14,14,15	0.58	0	15,19,21	1.42	1 (6%)
4	GLC	A	306	4	11,11,12	0.38	0	14,15,17	0.78	0
4	MAN	A	307	4	11,11,12	0.82	0	14,15,17	2.84	5 (35%)
4	MAN	A	308	4	11,11,12	1.33	2 (18%)	14,15,17	3.85	6 (42%)
5	NAG	A	309	1,5	14,14,15	0.53	0	15,19,21	0.92	1 (6%)
5	NAG	A	310	5	14,14,15	0.57	0	15,19,21	1.69	1 (6%)
5	GLC	A	311	5	11,11,12	0.38	0	14,15,17	0.79	0
5	BMA	A	312	5	11,11,12	0.57	0	14,15,17	2.42	4 (28%)
5	MAN	A	313	5	11,11,12	0.41	0	14,15,17	1.20	1 (7%)
5	FUC	A	314	5	10,10,11	0.62	0	14,14,16	1.04	0
7	BGC	A	316	7,6	11,11,12	1.32	1 (9%)	14,15,17	1.78	4 (28%)
7	GAL	A	317	7	11,11,12	1.55	3 (27%)	14,15,17	1.50	3 (21%)

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
4	NAG	A	304	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	305	4	-	0/6/23/26	0/1/1/1
4	GLC	A	306	4	-	0/2/19/22	0/1/1/1
4	MAN	A	307	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	308	4	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	A	309	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	310	5	-	0/6/23/26	0/1/1/1
5	GLC	A	311	5	1/1/4/5	0/2/19/22	0/1/1/1
5	BMA	A	312	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	313	5	-	0/2/19/22	0/1/1/1
5	FUC	A	314	5	-	0/0/17/20	0/1/1/1
7	BGC	A	316	7,6	-	0/2/19/22	0/1/1/1
7	GAL	A	317	7	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	308	MAN	O5-C1	-2.54	1.39	1.43
4	A	308	MAN	C1-C2	-2.39	1.46	1.52
7	A	317	GAL	O5-C1	2.03	1.47	1.43
7	A	317	GAL	C1-C2	2.35	1.57	1.52
7	A	317	GAL	C2-C3	2.47	1.55	1.52
7	A	316	BGC	O4-C4	2.70	1.49	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	308	MAN	C1-O5-C5	-9.60	100.07	112.25
4	A	307	MAN	C1-O5-C5	-6.07	104.54	112.25
4	A	308	MAN	C1-C2-C3	-5.91	102.55	109.54
5	A	312	BMA	C1-O5-C5	-5.83	104.84	112.25
4	A	307	MAN	C1-C2-C3	-5.72	102.77	109.54
5	A	312	BMA	C1-C2-C3	-4.57	104.14	109.54
4	A	305	NAG	C2-N2-C7	-4.50	117.26	123.04
5	A	313	MAN	C1-O5-C5	-3.66	107.60	112.25
4	A	308	MAN	O3-C3-C2	-3.29	104.06	110.00
4	A	307	MAN	O2-C2-C3	-2.78	104.52	110.12
7	A	316	BGC	O3-C3-C2	-2.46	105.56	110.00
7	A	317	GAL	C3-C4-C5	2.32	114.24	110.20
7	A	316	BGC	C3-C4-C5	2.45	114.47	110.20
7	A	317	GAL	C2-C3-C4	2.55	115.37	111.04
5	A	309	NAG	O5-C5-C6	2.57	112.91	107.35
4	A	308	MAN	O5-C5-C6	2.63	113.04	107.35
5	A	312	BMA	C3-C4-C5	2.70	114.90	110.20
4	A	307	MAN	C3-C4-C5	2.79	115.07	110.20
7	A	316	BGC	C1-C2-C3	2.90	112.97	109.54
7	A	316	BGC	C2-C3-C4	3.21	116.49	111.04
5	A	312	BMA	O5-C5-C6	3.51	114.95	107.35
7	A	317	GAL	C1-C2-C3	3.61	113.81	109.54
4	A	308	MAN	C2-C3-C4	3.86	117.60	111.04
4	A	307	MAN	O2-C2-C1	4.85	118.93	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	310	NAG	C1-O5-C5	5.71	119.50	112.25
4	A	308	MAN	O5-C1-C2	6.13	120.80	110.86

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	311	GLC	C1
4	A	307	MAN	C1
4	A	308	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	GLC	1	0
4	A	307	MAN	2	0
4	A	308	MAN	1	0
5	A	311	GLC	1	0
5	A	313	MAN	1	0

5.6 Ligand geometry [i](#)

2 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	NAG	A	303	1	14,14,15	0.70	0	15,19,21	0.97	1 (6%)
6	ERA	A	315	7	39,40,44	2.46	9 (23%)	37,42,46	2.47	7 (18%)

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	NAG	A	303	1	-	0/6/23/26	0/1/1/1
6	ERA	A	315	7	2/2/3/12	1/43/43/47	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	315	ERA	OAD-CAC	-9.86	1.23	1.43
6	A	315	ERA	CAB-NB	-7.30	1.33	1.46
6	A	315	ERA	CAC-CAE	-5.63	1.38	1.49
6	A	315	ERA	CBG-CBH	-2.25	1.40	1.50
6	A	315	ERA	CBT-CBS	-2.24	1.40	1.50
6	A	315	ERA	CBJ-CBI	-2.21	1.40	1.50
6	A	315	ERA	CBO-CBP	-2.17	1.40	1.50
6	A	315	ERA	CBR-CBS	2.61	1.40	1.32
6	A	315	ERA	CBQ-CBP	2.64	1.40	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	315	ERA	CAG-CAF-CAE	-5.28	109.31	125.14
6	A	315	ERA	CBD-CBC-CBB	-2.43	106.82	113.24
3	A	303	NAG	C4-C3-C2	2.83	115.64	111.23
6	A	315	ERA	OAD-CAC-CAE	3.06	119.36	110.78
6	A	315	ERA	CAB-NB-CBB	4.12	131.24	123.61
6	A	315	ERA	OA-CAA-CAB	4.89	124.21	111.12
6	A	315	ERA	OAD-CAC-CAB	5.60	122.93	107.94
6	A	315	ERA	CAA-CAB-NB	9.98	127.48	109.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	315	ERA	CAC
6	A	315	ERA	CAB

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	315	ERA	CAA-CAB-NB-CBB

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	267/302 (88%)	0.27	6 (2%) 65 69	34, 55, 92, 130	0
2	B	98/99 (98%)	0.13	1 (1%) 84 86	33, 50, 71, 79	0
All	All	365/401 (91%)	0.23	7 (1%) 70 73	33, 54, 86, 130	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ALA	3.1
1	A	93	ASP	2.8
2	B	99	MET	2.6
1	A	204	ARG	2.5
1	A	256	GLY	2.4
1	A	197	PRO	2.0
1	A	253	VAL	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
5	BMA	A	312	11/12	0.91	0.33	5.73	35,36,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MAN	A	307	11/12	0.80	0.26	3.51	27,28,29,29	0
4	NAG	A	304	14/15	0.87	0.18	0.45	22,24,26,27	0
5	FUC	A	314	10/11	0.92	0.17	0.05	29,31,31,33	0
5	NAG	A	309	14/15	0.93	0.14	-0.43	18,22,26,29	0
4	GLC	A	306	11/12	0.85	0.35	-	29,30,30,30	0
5	GLC	A	311	11/12	0.82	0.25	-	35,37,37,39	0
4	MAN	A	308	11/12	0.82	0.33	-	29,30,30,30	0
4	NAG	A	305	14/15	0.82	0.27	-	28,29,30,31	0
7	GAL	A	317	11/12	0.60	0.25	-	88,90,91,91	0
5	NAG	A	310	14/15	0.91	0.22	-	29,32,34,35	0
5	MAN	A	313	11/12	0.86	0.28	-	40,41,41,42	0
7	BGC	A	316	11/12	0.89	0.12	-	77,79,81,85	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
6	ERA	A	315	41/45	0.81	0.43	8.05	52,64,70,74	0
3	NAG	A	303	14/15	0.78	0.32	-	27,28,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.