



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:02 PM UTC

PDB ID : 4IQP / pdb_00004iqp
Title : Crystal Structure of HCRA-W1266A
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Deposited on : 2013-01-12
Resolution : 2.30 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

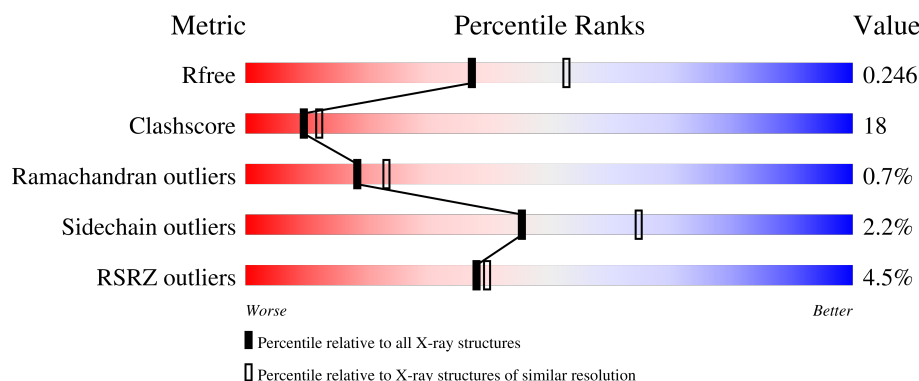
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	426	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1402	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3638 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.

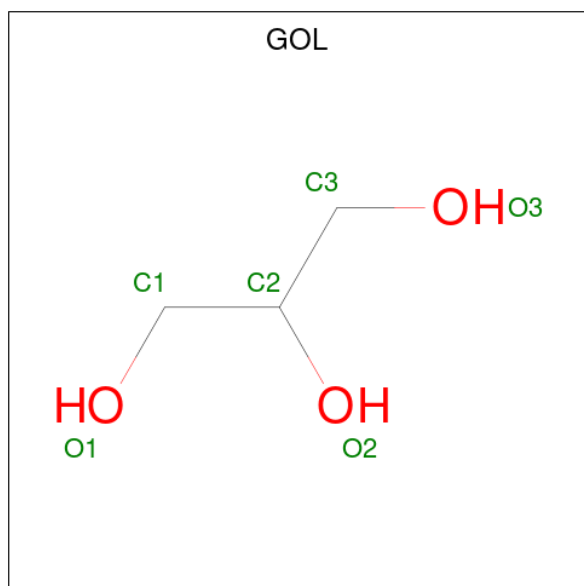
- Molecule 1 is a protein called Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3440	2191	594	642	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	ALA	TRP	engineered mutation	UNP P10845

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	A	1	6	3	3	0	0

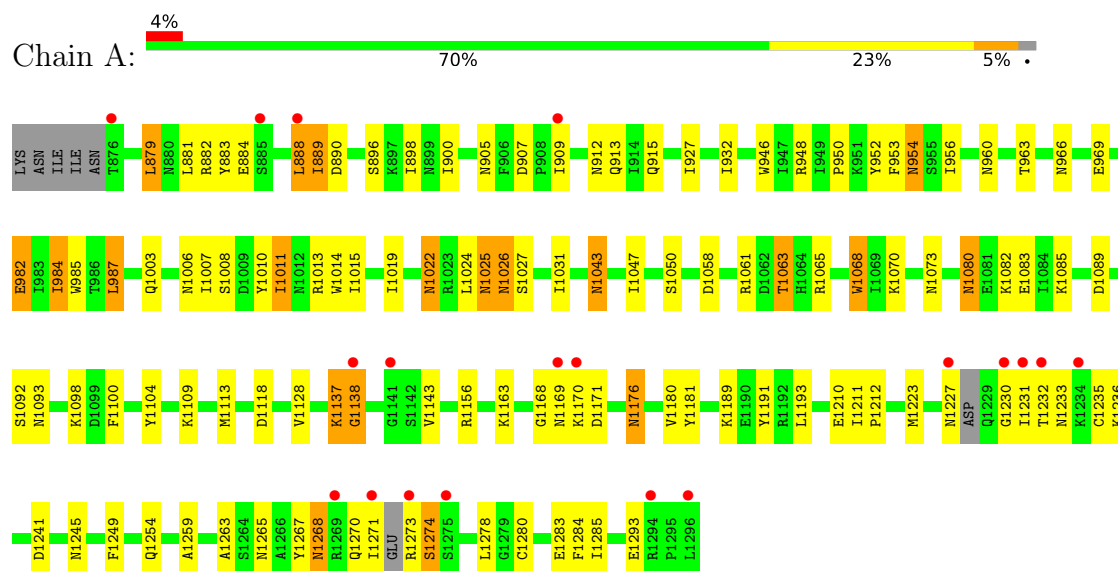
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total 186	O 186	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Botulinum neurotoxin type A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.15Å 80.63Å 138.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.32 – 2.30 40.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.3 (40.32-2.30) 93.4 (40.32-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 2.29Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.207 , 0.246 0.206 , 0.246	Depositor DCC
R_{free} test set	1036 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3638	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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, 0.333 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: GOL

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	0.38	0/3509	0.94	21/4739 (0.4%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1210	GLU	N-CA-C	-7.37	98.98	109.96
1	A	1026	ASN	N-CA-C	7.25	121.31	109.85
1	A	1010	TYR	N-CA-C	6.19	120.86	113.12
1	A	1011	ILE	N-CA-C	6.08	117.14	108.93
1	A	1263	ALA	N-CA-C	-5.98	98.66	108.41
1	A	1118	ASP	CA-C-N	5.97	125.65	119.56
1	A	1118	ASP	C-N-CA	5.97	125.65	119.56
1	A	953	PHE	N-CA-C	5.88	120.61	112.90
1	A	954	ASN	N-CA-C	5.88	116.85	108.74
1	A	932	ILE	N-CA-C	5.49	117.45	112.29
1	A	1137	LYS	N-CA-C	5.49	117.61	110.53
1	A	982	GLU	N-CA-C	5.48	117.40	109.07
1	A	1180	VAL	N-CA-C	5.47	115.20	108.53
1	A	889	ILE	N-CA-C	5.33	115.32	108.82
1	A	966	ASN	N-CA-C	5.13	117.32	109.07
1	A	1063	THR	N-CA-C	5.12	117.59	111.71
1	A	984	ILE	N-CA-C	5.09	115.91	108.53
1	A	1236	LYS	N-CA-C	5.08	120.10	112.94
1	A	1176	ASN	N-CA-C	5.06	121.58	110.80
1	A	1068	TRP	N-CA-C	-5.06	101.44	109.59
1	A	1027	SER	N-CA-C	-5.01	101.52	109.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3407	122	0
2	A	12	0	16	8	0
3	A	186	0	0	2	0
All	All	3638	0	3423	122	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 18.

All (122) 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:913:GLN:HE21	1:A:1070:LYS:HZ2	1.02	0.98
1:A:1025:ASN:HD22	1:A:1026:ASN:H	0.97	0.94
1:A:1025:ASN:ND2	1:A:1026:ASN:H	1.65	0.93
1:A:1025:ASN:HD22	1:A:1026:ASN:N	1.68	0.91
1:A:1100:PHE:HD1	1:A:1283:GLU:HG2	1.35	0.90
1:A:952:TYR:H	1:A:1003:GLN:HE22	1.20	0.88
1:A:882:ARG:HH12	1:A:1073:ASN:HD21	1.23	0.85
1:A:913:GLN:NE2	1:A:1070:LYS:HZ2	1.75	0.83
1:A:1268:ASN:H	1:A:1268:ASN:HD22	1.23	0.82
1:A:1231:ILE:HG13	1:A:1232:THR:H	1.45	0.81
1:A:1113:MET:HE1	1:A:1284:PHE:CD2	2.21	0.75
1:A:905:ASN:HD22	1:A:915:GLN:HE21	1.32	0.74
1:A:881:LEU:HD22	1:A:888:LEU:HD22	1.69	0.74
1:A:1227:ASN:HB2	1:A:1230:GLY:HA3	1.69	0.73
1:A:1231:ILE:HG13	1:A:1232:THR:N	2.03	0.73
1:A:1268:ASN:HD22	1:A:1268:ASN:N	1.87	0.72
1:A:1080:ASN:ND2	1:A:1083:GLU:H	1.91	0.69
1:A:1006:ASN:C	1:A:1007:ILE:HD12	2.17	0.69
1:A:1100:PHE:CD1	1:A:1283:GLU:HG2	2.24	0.68
1:A:982:GLU:HG3	1:A:984:ILE:HD11	1.76	0.67
1:A:960:ASN:HD21	1:A:1061:ARG:H	1.42	0.67
1:A:1022:ASN:HD22	1:A:1024:LEU:H	1.42	0.67
1:A:1254:GLN:NE2	1:A:1259:ALA:HB2	2.11	0.66
1:A:889:ILE:HA	1:A:898:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:ILE:HD12	1:A:900:ILE:N	2.14	0.63
1:A:1137:LYS:HG2	1:A:1138:GLY:N	2.14	0.63
1:A:1100:PHE:HD1	1:A:1283:GLU:CG	2.11	0.61
1:A:954:ASN:HD22	1:A:956:ILE:H	1.46	0.61
1:A:905:ASN:HD22	1:A:915:GLN:NE2	1.97	0.61
1:A:1043:ASN:H	1:A:1043:ASN:HD22	1.48	0.59
1:A:1176:ASN:O	1:A:1223:MET:O	2.21	0.59
1:A:896:SER:HB3	1:A:927:ILE:O	2.03	0.58
1:A:907:ASP:OD1	1:A:909:ILE:HG22	2.03	0.58
1:A:1249:PHE:HD2	1:A:1268:ASN:ND2	2.01	0.58
1:A:883:TYR:H	1:A:912:ASN:ND2	2.02	0.58
1:A:883:TYR:H	1:A:912:ASN:HD21	1.52	0.58
1:A:1022:ASN:HD22	1:A:1022:ASN:C	2.12	0.57
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.39	0.57
1:A:1254:GLN:HE22	1:A:1259:ALA:HB2	1.71	0.56
1:A:1063:THR:HG23	3:A:1560:HOH:O	2.06	0.55
1:A:987:LEU:HD22	1:A:1047:ILE:HD13	1.89	0.55
1:A:1080:ASN:C	1:A:1080:ASN:HD22	2.15	0.55
1:A:984:ILE:HD12	1:A:984:ILE:N	2.22	0.55
1:A:881:LEU:HD21	1:A:898:ILE:HD13	1.89	0.55
1:A:1022:ASN:ND2	1:A:1024:LEU:H	2.05	0.54
1:A:1113:MET:HE1	1:A:1284:PHE:HA	1.89	0.54
1:A:1270:GLN:HE21	1:A:1278:LEU:HD22	1.73	0.54
1:A:1137:LYS:O	1:A:1138:GLY:O	2.25	0.54
1:A:1100:PHE:HB2	1:A:1285:ILE:HG12	1.89	0.54
1:A:985:TRP:CE3	1:A:1019:ILE:HD13	2.43	0.53
1:A:1113:MET:CE	1:A:1284:PHE:HA	2.38	0.53
1:A:1137:LYS:HG2	1:A:1138:GLY:H	1.73	0.52
1:A:1241:ASP:OD2	1:A:1245:ASN:HB2	2.09	0.52
1:A:1043:ASN:H	1:A:1043:ASN:ND2	2.08	0.52
1:A:1156:ARG:NH1	1:A:1156:ARG:HB3	2.24	0.52
1:A:1235:CYS:HA	1:A:1280:CYS:O	2.10	0.52
1:A:1168:GLY:O	1:A:1170:LYS:HD2	2.11	0.51
1:A:1137:LYS:CG	1:A:1138:GLY:N	2.74	0.51
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.93	0.50
1:A:1170:LYS:HD2	1:A:1170:LYS:N	2.26	0.50
1:A:1270:GLN:NE2	1:A:1278:LEU:HD22	2.27	0.50
1:A:1137:LYS:CG	1:A:1138:GLY:H	2.24	0.50
1:A:1113:MET:HE1	1:A:1284:PHE:CG	2.47	0.50
1:A:1189:LYS:HD3	1:A:1191:TYR:OH	2.11	0.50
1:A:954:ASN:HD21	1:A:956:ILE:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:ASN:ND2	1:A:956:ILE:HG22	2.27	0.49
1:A:1189:LYS:HD3	1:A:1191:TYR:CZ	2.47	0.48
1:A:1015:ILE:CG2	1:A:1031:ILE:HG23	2.44	0.48
1:A:1231:ILE:CG1	1:A:1232:THR:N	2.76	0.47
1:A:960:ASN:ND2	1:A:1061:ARG:H	2.09	0.47
1:A:1193:LEU:C	1:A:1193:LEU:HD23	2.39	0.47
1:A:1143:VAL:HG11	1:A:1293:GLU:HG3	1.95	0.47
1:A:1022:ASN:HB3	1:A:1025:ASN:ND2	2.28	0.47
1:A:1008:SER:OG	1:A:1011:ILE:HG13	2.14	0.47
1:A:1267:TYR:O	1:A:1271:ILE:HG13	2.15	0.46
1:A:1080:ASN:HD22	1:A:1082:LYS:N	2.14	0.46
1:A:1231:ILE:CG1	1:A:1232:THR:H	2.20	0.46
1:A:946:TRP:CZ3	2:A:1401:GOL:H31	2.51	0.45
1:A:950:PRO:O	1:A:1065:ARG:NH2	2.49	0.45
1:A:1163:LYS:HB2	1:A:1181:TYR:HB2	1.98	0.45
1:A:1092:SER:HA	2:A:1401:GOL:H32	1.98	0.45
1:A:1273:ARG:O	1:A:1274:SER:HB2	2.17	0.45
1:A:1011:ILE:O	1:A:1013:ARG:HG3	2.16	0.45
1:A:1080:ASN:HD21	1:A:1083:GLU:H	1.62	0.45
1:A:969:GLU:HB2	1:A:1050:SER:HB2	1.99	0.45
1:A:1080:ASN:ND2	1:A:1080:ASN:C	2.75	0.44
1:A:1093:ASN:HB2	2:A:1402:GOL:C3	2.47	0.44
1:A:1211:ILE:HB	1:A:1212:PRO:HD3	2.00	0.44
1:A:1098:LYS:HE3	2:A:1402:GOL:H12	1.98	0.43
1:A:1249:PHE:CD2	1:A:1268:ASN:ND2	2.85	0.43
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.99	0.43
1:A:1093:ASN:HB2	2:A:1402:GOL:H32	1.99	0.43
1:A:1232:THR:HG22	1:A:1233:ASN:N	2.33	0.43
1:A:1085:LYS:NZ	1:A:1089:ASP:OD2	2.50	0.42
1:A:1093:ASN:CG	2:A:1402:GOL:O3	2.62	0.42
1:A:1268:ASN:H	1:A:1268:ASN:ND2	1.99	0.42
1:A:954:ASN:ND2	1:A:956:ILE:H	2.14	0.42
1:A:1169:ASN:ND2	1:A:1171:ASP:O	2.53	0.42
1:A:879:LEU:HD23	1:A:890:ASP:OD1	2.19	0.42
1:A:1100:PHE:CB	1:A:1285:ILE:HG12	2.50	0.42
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	2.02	0.42
1:A:881:LEU:HD22	1:A:888:LEU:CD2	2.43	0.42
1:A:1156:ARG:HB3	1:A:1156:ARG:HH11	1.84	0.42
1:A:1265:ASN:HD22	1:A:1265:ASN:HA	1.66	0.42
1:A:1080:ASN:HD22	1:A:1082:LYS:H	1.68	0.41
1:A:1080:ASN:HD21	1:A:1082:LYS:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:ASP:OD2	1:A:1171:ASP:C	2.63	0.41
1:A:1249:PHE:H	1:A:1268:ASN:HD21	1.68	0.41
1:A:1113:MET:CE	1:A:1284:PHE:CD2	3.00	0.41
1:A:1025:ASN:ND2	1:A:1026:ASN:N	2.42	0.41
1:A:1080:ASN:ND2	1:A:1082:LYS:HB3	2.35	0.41
1:A:946:TRP:HA	1:A:1015:ILE:O	2.21	0.41
1:A:1235:CYS:SG	1:A:1280:CYS:C	3.04	0.41
1:A:963:THR:HB	1:A:1058:ASP:HB3	2.03	0.40
1:A:1014:TRP:CH2	1:A:1068:TRP:HB3	2.56	0.40
1:A:1104:TYR:CE1	2:A:1402:GOL:H2	2.56	0.40
1:A:1098:LYS:CE	2:A:1402:GOL:H12	2.52	0.40
1:A:1007:ILE:HD12	1:A:1007:ILE:N	2.37	0.40
1:A:1089:ASP:O	1:A:1092:SER:HB2	2.21	0.40
1:A:1109:LYS:HE2	3:A:1504:HOH:O	2.21	0.40
1:A:1128:VAL:HG11	1:A:1191:TYR:CE2	2.57	0.40
1:A:1232:THR:CG2	1:A:1233:ASN:N	2.84	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	413/426 (97%)	386 (94%)	24 (6%)	3 (1%)	18 23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1138	GLY
1	A	1274	SER
1	A	884	GLU

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	366/392 (93%)	358 (98%)	8 (2%)	45 65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	879	LEU
1	A	888	LEU
1	A	987	LEU
1	A	1022	ASN
1	A	1025	ASN
1	A	1043	ASN
1	A	1080	ASN
1	A	1268	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	880	ASN
1	A	912	ASN
1	A	913	GLN
1	A	915	GLN
1	A	954	ASN
1	A	959	ASN
1	A	960	ASN
1	A	971	ASN
1	A	1003	GLN
1	A	1012	ASN
1	A	1022	ASN
1	A	1025	ASN
1	A	1043	ASN
1	A	1046	ASN
1	A	1051	ASN
1	A	1073	ASN
1	A	1080	ASN

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Mol	Chain	Res	Type
1	A	1090	ASN
1	A	1106	GLN
1	A	1147	ASN
1	A	1151	ASN
1	A	1253	HIS
1	A	1254	GLN
1	A	1256	ASN
1	A	1268	ASN
1	A	1270	GLN

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 [i](#)

There are no oligosaccharides in this entry.

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	$\# Z > 2$
2	GOL	A	1401	-	5,5,5	0.66	0	5,5,5	0.77	0
2	GOL	A	1402	-	5,5,5	0.58	0	5,5,5	0.60	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
2	GOL	A	1401	-	-	0/4/4/4	-
2	GOL	A	1402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1402	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	GOL	2	0
2	A	1402	GOL	6	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	419/426 (98%)	0.05	19 (4%) 38 40	14, 25, 53, 73	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1231	ILE	5.3
1	A	876	THR	4.9
1	A	1138	GLY	3.5
1	A	1271	ILE	3.3
1	A	1296	LEU	3.3
1	A	1230	GLY	3.3
1	A	1232	THR	3.2
1	A	1170	LYS	3.1
1	A	1227	ASN	3.0
1	A	1269	ARG	2.8
1	A	885	SER	2.8
1	A	1141	GLY	2.5
1	A	1169	ASN	2.4
1	A	1275	SER	2.3
1	A	1273	ARG	2.2
1	A	909	ILE	2.1
1	A	888	LEU	2.0
1	A	1234	LYS	2.0
1	A	1294	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	1402	6/6	0.72	0.28	30,33,33,34	0
2	GOL	A	1401	6/6	0.88	0.12	30,33,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.