



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2021 – 08:04 PM EST

PDB ID : 7T9W  
Title : Crystal structure of the Nsp3 bSM (Betacoronavirus-Specific Marker) domain from SARS-CoV-2  
Authors : Stogios, P.J.; Skarina, T.; Di Leo, R.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2021-12-20  
Resolution : 2.20 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.25

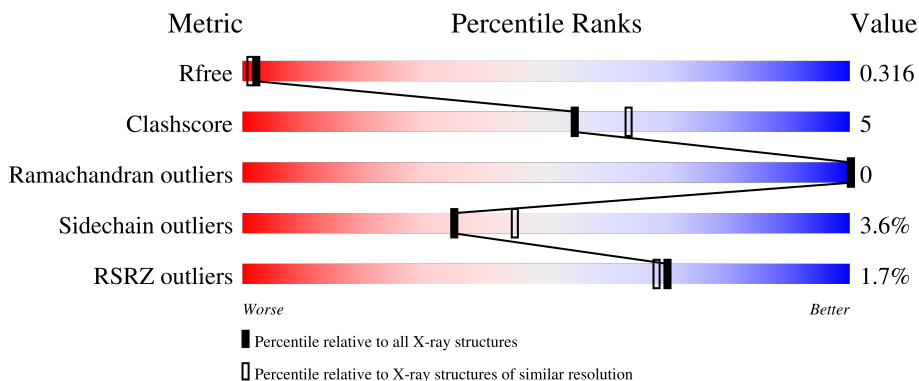
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	105	 5% 71% 12% 16%
1	B	105	 3% 78% 9% 12%
1	C	105	 % 76% 10% 14%
1	D	105	 73% 10% 15%
1	E	105	 67% 17% 15%

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Mol	Chain	Length	Quality of chain
1	F	105	<p>7% 62% 20% 13%</p>
1	G	105	<p>% 79% 7% 14%</p>
1	H	105	<p>73% 12% 13%</p>
1	I	105	<p>% 75% 9% 16%</p>
1	J	105	<p>69% 14% 15%</p>
1	K	105	<p>2% 66% 16% 15%</p>
1	L	105	<p>73% 10% 16%</p>
1	M	105	<p>2% 78% 8% 14%</p>
1	N	105	<p>2% 70% 13% 14%</p>
1	O	105	<p>% 71% 14% 14%</p>
1	P	105	<p>74% 10% 15%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11883 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.

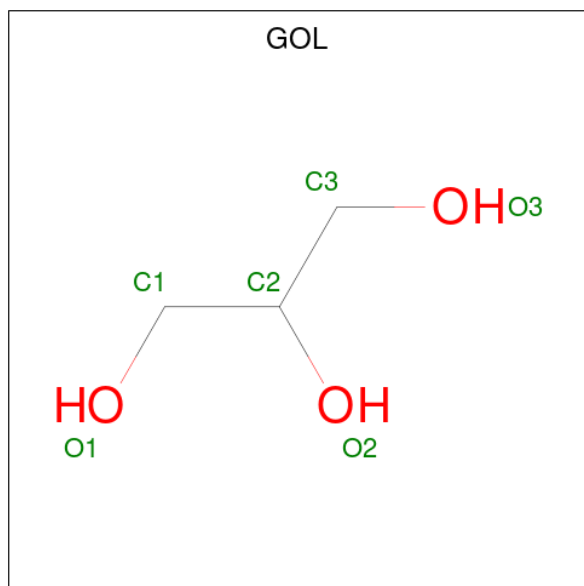
- Molecule 1 is a protein called Papain-like protease nsp3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	88	Total 673	C 430	N 111	O 130	S 2	0	1	0
1	B	92	Total 700	C 444	N 117	O 137	S 2	0	0	0
1	C	90	Total 685	C 434	N 115	O 134	S 2	0	0	0
1	D	89	Total 677	C 430	N 113	O 132	S 2	0	0	0
1	E	89	Total 677	C 430	N 113	O 132	S 2	0	0	0
1	F	88	Total 668	C 425	N 111	O 130	S 2	0	0	0
1	G	90	Total 685	C 434	N 115	O 134	S 2	0	0	0
1	H	91	Total 693	C 440	N 116	O 135	S 2	0	0	0
1	I	88	Total 668	C 425	N 111	O 130	S 2	0	0	0
1	J	89	Total 677	C 430	N 113	O 132	S 2	0	0	0
1	K	89	Total 677	C 430	N 113	O 132	S 2	0	0	0
1	L	88	Total 668	C 425	N 111	O 130	S 2	0	0	0
1	M	90	Total 685	C 436	N 114	O 133	S 2	0	0	0
1	N	90	Total 685	C 434	N 115	O 134	S 2	0	0	0
1	O	90	Total 685	C 434	N 115	O 134	S 2	0	0	0
1	P	89	Total 676	C 429	N 113	O 132	S 2	0	0	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	45	Total O 45 45	0	0
4	B	69	Total O 73 73	0	4
4	C	65	Total O 68 68	0	3
4	D	76	Total O 77 77	0	1
4	E	48	Total O 50 50	0	2
4	F	21	Total O 21 21	0	0

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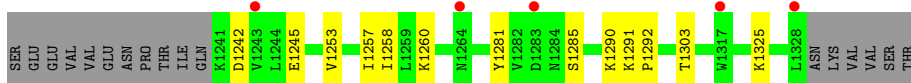
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	G	67	Total O 67 67	0	0
4	H	84	Total O 87 87	0	2
4	I	67	Total O 68 68	0	1
4	J	56	Total O 57 57	0	1
4	K	37	Total O 38 38	0	1
4	L	53	Total O 55 55	0	2
4	M	91	Total O 92 92	0	1
4	N	75	Total O 75 75	0	0
4	O	40	Total O 40 40	0	0
4	P	78	Total O 78 78	0	0

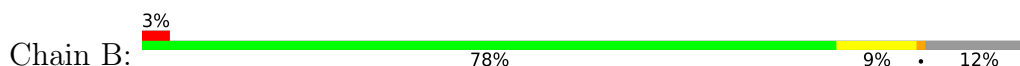
### 3 Residue-property plots [i](#)

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.

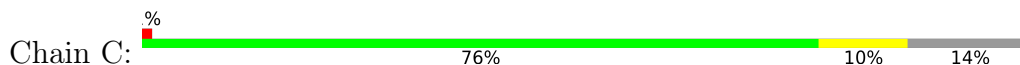
- Molecule 1: Papain-like protease nsp3



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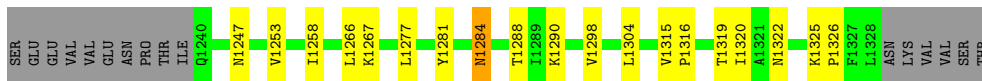
- Molecule 1: Papain-like protease nsp3



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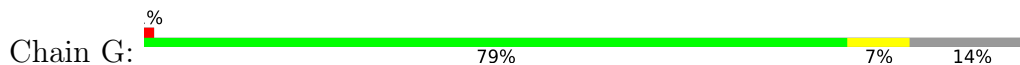


- Molecule 1: Papain-like protease nsp3



SER  
THR

- Molecule 1: Papain-like protease nsp3



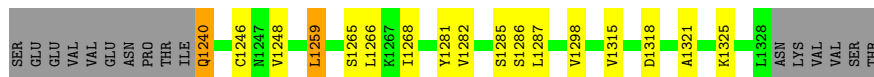
- Molecule 1: Papain-like protease nsp3



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- Molecule 1: Papain-like protease nsp3



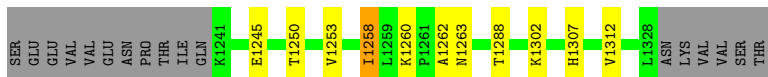
- Molecule 1: Papain-like protease nsp3



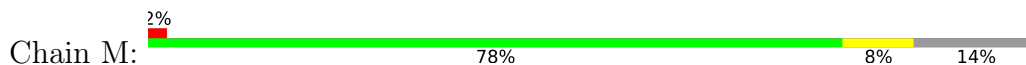
- Molecule 1: Papain-like protease nsp3







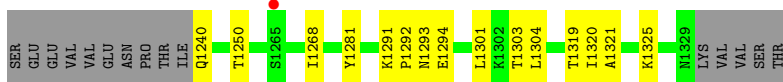
● Molecule 1: Papain-like protease nsp3



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● Molecule 1: Papain-like protease nsp3



● Molecule 1: Papain-like protease nsp3



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.46Å 157.46Å 79.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 2.20 29.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.42-2.20) 95.5 (29.42-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.262 , 0.316 0.263 , 0.316	Depositor DCC
$R_{free}$ test set	1982 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7922e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.23	0/686	0.46	0/935
1	B	0.24	0/710	0.45	0/968
1	C	0.24	0/695	0.45	0/947
1	D	0.28	0/687	0.46	0/936
1	E	0.24	0/687	0.45	0/936
1	F	0.25	0/678	0.49	0/924
1	G	0.24	0/695	0.46	0/947
1	H	0.24	0/703	0.45	0/958
1	I	0.24	0/678	0.47	0/924
1	J	0.25	0/687	0.48	0/936
1	K	0.30	0/687	0.51	0/936
1	L	0.26	0/678	0.45	0/924
1	M	0.24	0/695	0.45	0/947
1	N	0.25	0/695	0.49	0/947
1	O	0.24	0/695	0.45	0/947
1	P	0.23	0/686	0.44	0/935
All	All	0.25	0/11042	0.46	0/15047

There are no bond length outliers.

There are no bond angle outliers.

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	673	0	702	6	0
1	B	700	0	723	7	0
1	C	685	0	705	5	0
1	D	677	0	699	7	0
1	E	677	0	699	11	0
1	F	668	0	691	11	0
1	G	685	0	705	5	0
1	H	693	0	716	8	0
1	I	668	0	691	4	0
1	J	677	0	699	10	0
1	K	677	0	699	12	0
1	L	668	0	691	7	0
1	M	685	0	710	4	0
1	N	685	0	705	7	0
1	O	685	0	705	10	0
1	P	676	0	697	5	0
2	B	1	0	0	1	0
3	D	6	0	8	0	0
3	H	6	0	8	0	0
4	A	45	0	0	0	0
4	B	73	0	0	1	0
4	C	68	0	0	0	0
4	D	77	0	0	1	0
4	E	50	0	0	1	0
4	F	21	0	0	0	0
4	G	67	0	0	0	0
4	H	87	0	0	2	0
4	I	68	0	0	1	0
4	J	57	0	0	1	0
4	K	38	0	0	1	0
4	L	55	0	0	0	0
4	M	92	0	0	1	0
4	N	75	0	0	0	0
4	O	40	0	0	2	0
4	P	78	0	0	1	0
All	All	11883	0	11253	114	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 5.

All (114) 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:J:1240:GLN:HE21	1:J:1240:GLN:N	1.85	0.75
1:F:1242:ASP:N	1:F:1242:ASP:OD1	2.23	0.72
1:E:1322:ASN:HA	1:E:1325:LYS:HE2	1.74	0.69
1:C:1241:LYS:HE3	1:C:1258:ILE:HD11	1.74	0.69
1:F:1287:LEU:HB2	1:F:1315:VAL:HG21	1.79	0.64
1:B:1253:VAL:HG22	1:B:1258:ILE:HG12	1.81	0.62
1:F:1285:SER:OG	1:F:1286:SER:N	2.35	0.59
1:A:1290:LYS:HG2	1:A:1291:LYS:HG3	1.86	0.58
1:K:1242:ASP:HB2	1:K:1257:ILE:HG22	1.87	0.56
1:K:1268:ILE:HD13	1:K:1304:LEU:HD11	1.87	0.55
1:N:1242:ASP:HB2	1:N:1257:ILE:HG22	1.88	0.55
1:B:1325:LYS:NZ	4:B:1503:HOH:O	2.39	0.54
1:O:1291:LYS:NZ	4:O:1406:HOH:O	2.42	0.53
1:K:1272:VAL:HB	1:K:1289:ILE:HD13	1.91	0.53
1:D:1242:ASP:HB2	1:D:1257:ILE:HG22	1.91	0.53
1:E:1298:VAL:HG12	1:L:1250:THR:HG23	1.91	0.52
1:O:1321:ALA:O	1:O:1325:LYS:HG2	2.10	0.52
1:D:1290:LYS:HG3	1:D:1291:LYS:HG3	1.92	0.51
1:P:1241:LYS:NZ	4:P:1405:HOH:O	2.43	0.51
1:J:1325:LYS:NZ	4:J:1407:HOH:O	2.44	0.50
1:O:1293:ASN:N	1:O:1293:ASN:OD1	2.43	0.50
1:B:1242:ASP:HB2	1:B:1257:ILE:HG22	1.93	0.49
1:O:1301:LEU:HD21	1:O:1319:THR:HG21	1.94	0.49
1:L:1245:GLU:HB3	1:L:1260:LYS:HD2	1.94	0.49
1:D:1249:LYS:NZ	4:D:1509:HOH:O	2.41	0.49
1:A:1242:ASP:HB2	1:A:1257:ILE:HG22	1.94	0.49
1:A:1253:VAL:HG22	1:A:1258:ILE:HG12	1.93	0.49
1:H:1302:LYS:HG2	1:H:1307:HIS:CD2	2.48	0.49
1:K:1325:LYS:HG3	1:K:1326:PRO:HD3	1.93	0.49
1:N:1321:ALA:O	1:N:1325:LYS:HG2	2.12	0.49
1:K:1302:LYS:HE2	1:K:1314:SER:HB2	1.94	0.49
1:O:1281:TYR:HB2	1:O:1320:ILE:HG22	1.95	0.48
1:E:1253:VAL:HG12	1:E:1258:ILE:HD12	1.95	0.48
1:I:1291:LYS:NZ	4:I:1405:HOH:O	2.47	0.48
1:J:1281:TYR:HD2	1:J:1321:ALA:HA	1.77	0.48
1:J:1282:VAL:HG22	1:L:1258:ILE:HG21	1.94	0.48
1:K:1321:ALA:O	1:K:1325:LYS:HG2	2.13	0.48
1:E:1281:TYR:HB2	1:E:1320:ILE:HG22	1.96	0.48
1:J:1248:VAL:HG11	1:J:1259:LEU:HD23	1.95	0.48
1:G:1246:CYS:HA	1:G:1265:SER:HB3	1.96	0.48
1:C:1279:ALA:HA	1:G:1260:LYS:HE3	1.96	0.48
1:O:1240:GLN:N	4:O:1408:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1302:LYS:NZ	4:H:1509:HOH:O	2.46	0.47
1:F:1293:ASN:H	1:F:1296:SER:HG	1.61	0.47
1:J:1246:CYS:HB2	1:J:1268:ILE:HD11	1.95	0.47
1:M:1284:ASN:ND2	4:M:1410:HOH:O	2.45	0.47
1:C:1321:ALA:O	1:C:1325:LYS:HG2	2.15	0.47
1:O:1268:ILE:HD13	1:O:1304:LEU:HD11	1.97	0.47
1:D:1287:LEU:HB2	1:D:1315:VAL:HG21	1.96	0.47
1:A:1292:PRO:HB3	1:A:1303:THR:HG21	1.97	0.47
1:N:1246:CYS:HA	1:N:1265:SER:HB3	1.97	0.47
1:L:1253:VAL:HG22	1:L:1258:ILE:HD11	1.98	0.46
1:P:1266:LEU:HD21	1:P:1312:VAL:HG13	1.98	0.46
1:E:1315:VAL:HG11	1:E:1320:ILE:HD11	1.97	0.46
1:F:1247:ASN:HB2	1:F:1266:LEU:O	2.15	0.46
1:G:1260:LYS:HD3	1:G:1261:PRO:HD2	1.97	0.46
1:H:1301:LEU:HD22	1:H:1315:VAL:HG13	1.97	0.46
1:A:1281:TYR:OH	1:A:1325:LYS:NZ	2.49	0.46
1:J:1286:SER:OG	1:J:1315:VAL:O	2.34	0.46
1:K:1264:ASN:OD1	1:K:1264:ASN:N	2.45	0.46
1:J:1246:CYS:SG	1:J:1268:ILE:HD11	2.56	0.45
1:K:1257:ILE:HG21	1:K:1309:LEU:HD23	1.98	0.45
1:J:1265:SER:HB3	1:J:1266:LEU:H	1.65	0.45
1:L:1302:LYS:HB3	1:L:1307:HIS:CG	2.52	0.45
1:C:1250:THR:HA	1:O:1294:GLU:HG3	1.98	0.45
1:F:1301:LEU:HD21	1:F:1315:VAL:HG13	1.98	0.45
1:H:1281:TYR:HB2	1:H:1320:ILE:HG22	1.98	0.45
1:E:1290:LYS:HA	1:E:1304:LEU:HB2	1.98	0.45
1:K:1251:THR:HA	1:K:1259:LEU:O	2.17	0.45
1:L:1288:THR:HG23	1:L:1312:VAL:HA	1.98	0.45
1:D:1244:LEU:HD11	1:D:1266:LEU:HD12	1.99	0.44
1:E:1284:ASN:ND2	4:E:1405:HOH:O	2.48	0.44
1:B:1241:LYS:HE3	2:B:1401:CL:CL	2.55	0.44
1:K:1302:LYS:NZ	4:K:1402:HOH:O	2.48	0.44
1:E:1325:LYS:HB2	1:E:1326:PRO:HD3	1.99	0.44
1:F:1245:GLU:HB2	1:F:1262:ALA:HB2	2.00	0.44
1:F:1257:ILE:HD12	1:F:1257:ILE:HA	1.86	0.44
1:M:1252:GLU:OE1	1:M:1290:LYS:NZ	2.39	0.43
1:L:1245:GLU:HB2	1:L:1262:ALA:HB2	2.00	0.43
1:J:1287:LEU:HB2	1:J:1315:VAL:HG21	2.00	0.43
1:B:1294:GLU:HG3	1:O:1250:THR:HG22	2.00	0.43
1:H:1246:CYS:HA	1:H:1265:SER:HB3	2.01	0.43
1:M:1301:LEU:HD22	1:M:1315:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1281:TYR:HB2	1:P:1320:ILE:HG22	2.01	0.43
1:F:1246:CYS:SG	1:F:1248:VAL:HG23	2.59	0.43
1:C:1248:VAL:HG21	1:C:1259:LEU:HB3	2.01	0.43
1:B:1239:ILE:HD12	1:B:1239:ILE:HA	1.91	0.42
1:E:1247:ASN:ND2	1:E:1267:LYS:HD2	2.34	0.42
1:E:1316:PRO:HG2	1:E:1319:THR:OG1	2.20	0.42
1:I:1287:LEU:HB2	1:I:1315:VAL:HG21	2.01	0.42
1:F:1284:ASN:HA	1:F:1317:TRP:CH2	2.55	0.42
1:N:1241:LYS:HB3	1:N:1256:ASP:O	2.18	0.42
1:H:1241:LYS:HD2	1:H:1258:ILE:HD11	2.01	0.42
1:N:1251:THR:HG22	1:N:1258:ILE:HD11	2.00	0.42
1:N:1287:LEU:HB2	1:N:1315:VAL:HG21	2.00	0.42
1:O:1292:PRO:HB3	1:O:1303:THR:HG21	2.02	0.42
1:H:1302:LYS:HG2	1:H:1307:HIS:CG	2.55	0.42
1:K:1246:CYS:SG	1:K:1259:LEU:HB3	2.59	0.42
1:P:1293:ASN:O	1:P:1297:ARG:HG3	2.19	0.42
1:E:1266:LEU:HD21	1:E:1288:THR:HG21	2.02	0.41
1:F:1281:TYR:HB2	1:F:1320:ILE:HG22	2.01	0.41
1:G:1260:LYS:HD3	1:G:1261:PRO:CD	2.50	0.41
1:M:1242:ASP:HB2	1:M:1257:ILE:HG22	2.01	0.41
1:N:1242:ASP:HB3	1:N:1309:LEU:HD11	2.02	0.41
1:A:1245:GLU:HG2	1:A:1260:LYS:HD3	2.02	0.41
1:B:1241:LYS:HD2	1:B:1258:ILE:HG13	2.01	0.41
1:I:1281:TYR:HD2	1:I:1321:ALA:HA	1.85	0.41
1:D:1246:CYS:SG	1:D:1259:LEU:HB3	2.61	0.41
1:P:1301:LEU:HD22	1:P:1315:VAL:HG13	2.02	0.41
1:H:1291:LYS:NZ	4:H:1507:HOH:O	2.36	0.40
1:I:1242:ASP:HB2	1:I:1257:ILE:HG22	2.04	0.40
1:K:1290:LYS:HA	1:K:1304:LEU:HD12	2.03	0.40
1:D:1290:LYS:HG3	1:D:1291:LYS:N	2.36	0.40
1:G:1249:LYS:HA	1:G:1249:LYS:HD3	1.95	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	87/105 (83%)	83 (95%)	4 (5%)	0	100	100
1	B	90/105 (86%)	87 (97%)	3 (3%)	0	100	100
1	C	88/105 (84%)	84 (96%)	4 (4%)	0	100	100
1	D	87/105 (83%)	85 (98%)	2 (2%)	0	100	100
1	E	87/105 (83%)	82 (94%)	5 (6%)	0	100	100
1	F	86/105 (82%)	80 (93%)	6 (7%)	0	100	100
1	G	88/105 (84%)	87 (99%)	1 (1%)	0	100	100
1	H	89/105 (85%)	89 (100%)	0	0	100	100
1	I	86/105 (82%)	84 (98%)	2 (2%)	0	100	100
1	J	87/105 (83%)	84 (97%)	3 (3%)	0	100	100
1	K	87/105 (83%)	83 (95%)	4 (5%)	0	100	100
1	L	86/105 (82%)	85 (99%)	1 (1%)	0	100	100
1	M	88/105 (84%)	85 (97%)	3 (3%)	0	100	100
1	N	88/105 (84%)	84 (96%)	4 (4%)	0	100	100
1	O	88/105 (84%)	85 (97%)	3 (3%)	0	100	100
1	P	87/105 (83%)	81 (93%)	6 (7%)	0	100	100
All	All	1399/1680 (83%)	1348 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	77/93 (83%)	76 (99%)	1 (1%)	69	81
1	B	80/93 (86%)	77 (96%)	3 (4%)	33	42
1	C	78/93 (84%)	76 (97%)	2 (3%)	46	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	77/93 (83%)	75 (97%)	2 (3%)	46	58
1	E	77/93 (83%)	75 (97%)	2 (3%)	46	58
1	F	76/93 (82%)	70 (92%)	6 (8%)	12	12
1	G	78/93 (84%)	76 (97%)	2 (3%)	46	58
1	H	79/93 (85%)	75 (95%)	4 (5%)	24	29
1	I	76/93 (82%)	74 (97%)	2 (3%)	46	58
1	J	77/93 (83%)	72 (94%)	5 (6%)	17	19
1	K	77/93 (83%)	71 (92%)	6 (8%)	12	13
1	L	76/93 (82%)	74 (97%)	2 (3%)	46	58
1	M	78/93 (84%)	77 (99%)	1 (1%)	69	81
1	N	78/93 (84%)	73 (94%)	5 (6%)	17	20
1	O	78/93 (84%)	78 (100%)	0	100	100
1	P	77/93 (83%)	75 (97%)	2 (3%)	46	58
All	All	1239/1488 (83%)	1194 (96%)	45 (4%)	35	45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1285	SER
1	B	1239	ILE
1	B	1266	LEU
1	B	1267	LYS
1	C	1318	ASP
1	C	1329	ASN
1	D	1264	ASN
1	D	1290	LYS
1	E	1277	LEU
1	E	1284	ASN
1	F	1242	ASP
1	F	1266	LEU
1	F	1294	GLU
1	F	1313	ASN
1	F	1314	SER
1	F	1319	THR
1	G	1267	LYS
1	G	1329	ASN
1	H	1265	SER

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Mol	Chain	Res	Type
1	H	1266	LEU
1	H	1317	TRP
1	H	1329	ASN
1	I	1241	LYS
1	I	1318	ASP
1	J	1240	GLN
1	J	1259	LEU
1	J	1285	SER
1	J	1298	VAL
1	J	1318	ASP
1	K	1258	ILE
1	K	1264	ASN
1	K	1268	ILE
1	K	1285	SER
1	K	1301	LEU
1	K	1309	LEU
1	L	1258	ILE
1	L	1263	ASN
1	M	1272	VAL
1	N	1241	LYS
1	N	1265	SER
1	N	1269	THR
1	N	1281	TYR
1	N	1302	LYS
1	P	1249	LYS
1	P	1284	ASN

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
3	GOL	H	1401	-	5,5,5	0.91	0	5,5,5	1.01	0
3	GOL	D	1401	-	5,5,5	0.92	0	5,5,5	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	H	1401	-	-	0/4/4/4	-
3	GOL	D	1401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 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, 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	88/105 (83%)	0.11	5 (5%) 23 22	43, 62, 94, 114	0
1	B	92/105 (87%)	-0.30	3 (3%) 46 44	32, 48, 82, 119	0
1	C	90/105 (85%)	-0.21	1 (1%) 80 79	34, 50, 76, 103	0
1	D	89/105 (84%)	-0.45	0 100 100	36, 43, 62, 91	0
1	E	89/105 (84%)	0.04	0 100 100	45, 65, 86, 99	0
1	F	88/105 (83%)	0.57	7 (7%) 12 11	58, 90, 113, 146	0
1	G	90/105 (85%)	-0.33	1 (1%) 80 79	30, 46, 71, 102	0
1	H	91/105 (86%)	-0.49	0 100 100	26, 36, 63, 98	0
1	I	88/105 (83%)	-0.29	1 (1%) 80 79	33, 47, 72, 97	0
1	J	89/105 (84%)	-0.30	0 100 100	41, 54, 78, 108	0
1	K	89/105 (84%)	-0.00	2 (2%) 62 59	43, 67, 99, 138	0
1	L	88/105 (83%)	-0.25	0 100 100	31, 56, 80, 105	0
1	M	90/105 (85%)	-0.32	2 (2%) 62 59	30, 39, 66, 118	0
1	N	90/105 (85%)	-0.34	2 (2%) 62 59	36, 47, 78, 112	0
1	O	90/105 (85%)	-0.07	1 (1%) 80 79	38, 61, 83, 118	0
1	P	89/105 (84%)	-0.26	0 100 100	29, 51, 71, 92	0
All	All	1430/1680 (85%)	-0.18	25 (1%) 70 68	26, 53, 95, 146	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1310	ALA	8.0
1	M	1240	GLN	4.1
1	K	1310	ALA	3.8
1	F	1311	ALA	3.6
1	A	1243	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	O	1265	SER	3.5
1	B	1239	ILE	3.4
1	B	1317	TRP	3.1
1	A	1317	TRP	2.9
1	C	1264	ASN	2.8
1	G	1264	ASN	2.8
1	B	1238	THR	2.7
1	F	1243	VAL	2.6
1	I	1264	ASN	2.6
1	N	1329	ASN	2.6
1	F	1254	VAL	2.5
1	M	1239	ILE	2.4
1	F	1245	GLU	2.4
1	F	1255	GLY	2.4
1	K	1264	ASN	2.3
1	A	1264	ASN	2.2
1	F	1317	TRP	2.2
1	A	1328	LEU	2.2
1	A	1283	ASP	2.2
1	N	1317	TRP	2.2

## 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](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	H	1401	6/6	0.70	0.21	61,63,67,72	0
2	CL	B	1401	1/1	0.87	0.09	79,79,79,79	0
3	GOL	D	1401	6/6	0.88	0.16	51,55,56,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.