



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:23 am BST

PDB ID : 2OJ5  
Title : Crystal Structure of Reovirus T3D Attachment Protein Sigma1 head domain wild-type at 1.75 Å resolution  
Authors : Stehle, T.; Schelling, P.; Kirchner, E.; Dermody, T.S.  
Deposited on : 2007-01-12  
Resolution : 1.75 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 : 2.11  
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) : 2.11

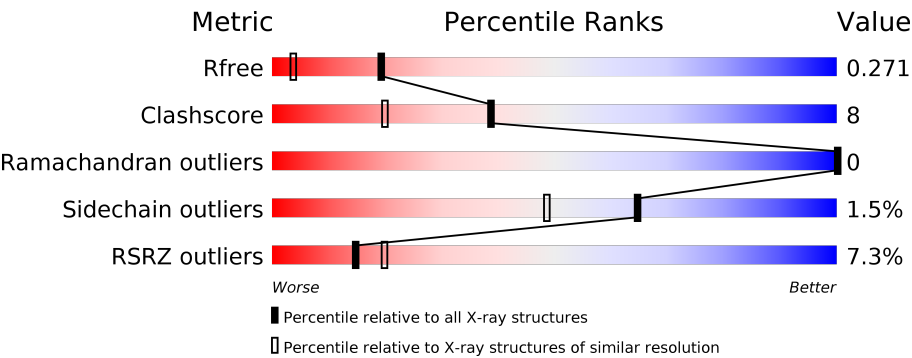
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	165	
1	B	165	
1	C	165	
1	D	165	
1	E	165	
1	F	165	

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
3	GOL	B	2500	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8851 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 Viral attachment protein sigma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	3	0
			1265	808	212	240	5			
1	B	163	Total	C	N	O	S	0	4	0
			1280	815	215	245	5			
1	C	162	Total	C	N	O	S	0	6	0
			1292	825	219	243	5			
1	D	160	Total	C	N	O	S	0	8	0
			1299	825	224	245	5			
1	E	161	Total	C	N	O	S	0	4	0
			1273	814	216	238	5			
1	F	163	Total	C	N	O	S	0	2	0
			1269	808	213	243	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLY	-	CLONING ARTIFACT	UNP Q86337
A	292	SER	-	CLONING ARTIFACT	UNP Q86337
B	291	GLY	-	CLONING ARTIFACT	UNP Q86337
B	292	SER	-	CLONING ARTIFACT	UNP Q86337
C	291	GLY	-	CLONING ARTIFACT	UNP Q86337
C	292	SER	-	CLONING ARTIFACT	UNP Q86337
D	291	GLY	-	CLONING ARTIFACT	UNP Q86337
D	292	SER	-	CLONING ARTIFACT	UNP Q86337
E	291	GLY	-	CLONING ARTIFACT	UNP Q86337
E	292	SER	-	CLONING ARTIFACT	UNP Q86337
F	291	GLY	-	CLONING ARTIFACT	UNP Q86337
F	292	SER	-	CLONING ARTIFACT	UNP Q86337

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

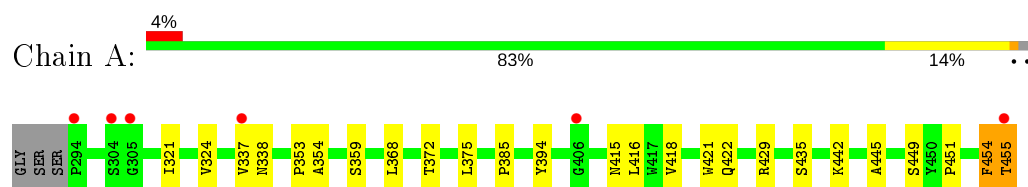
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	184	Total	O	0	0
			184	184		
4	C	193	Total	O	0	0
			193	193		
4	D	203	Total	O	0	0
			203	203		
4	E	195	Total	O	0	0
			195	195		
4	F	176	Total	O	0	0
			176	176		

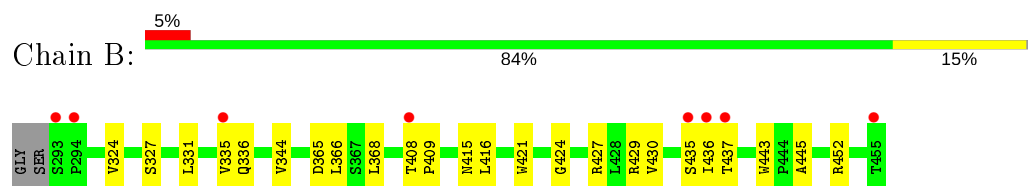
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

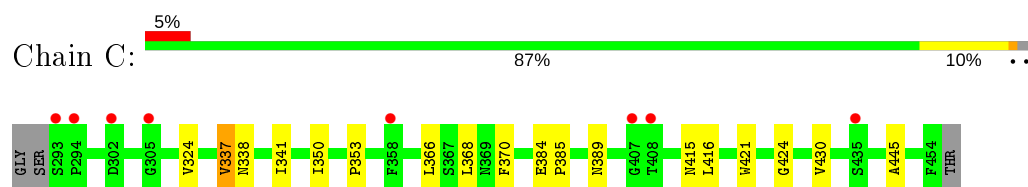
- Molecule 1: Viral attachment protein sigma 1



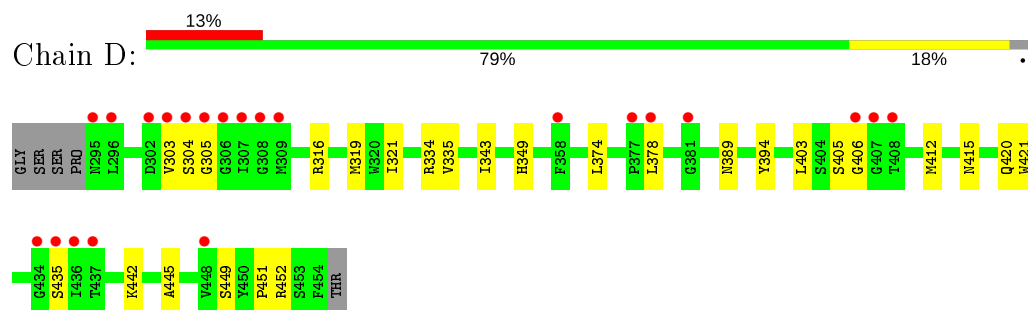
- Molecule 1: Viral attachment protein sigma 1



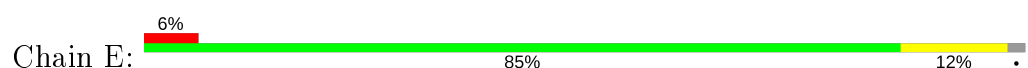
- Molecule 1: Viral attachment protein sigma 1

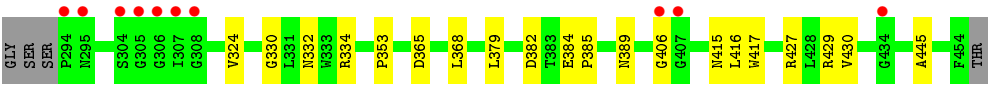


- Molecule 1: Viral attachment protein sigma 1

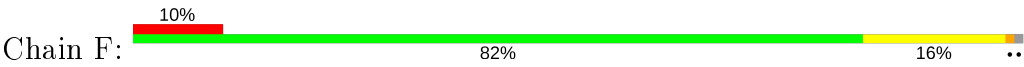


- Molecule 1: Viral attachment protein sigma 1





● Molecule 1: Viral attachment protein sigma 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.93Å 51.38Å 108.87Å 90.00° 95.66° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 43.76 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-1.75) 96.6 (43.76-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	9.30	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.228 , 0.274 0.226 , 0.271	Depositor DCC
$R_{free}$ test set	9050 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG

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	0.39	0/1304	0.49	0/1778
1	B	0.37	0/1316	0.48	0/1795
1	C	0.39	0/1328	0.46	0/1812
1	D	0.51	4/1334 (0.3%)	0.51	0/1817
1	E	0.47	2/1309 (0.2%)	0.46	0/1785
1	F	0.49	2/1305 (0.2%)	0.51	0/1780
All	All	0.44	8/7896 (0.1%)	0.48	0/10767

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
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	406	GLY	C-N	8.42	1.48	1.33
1	E	406	GLY	N-CA	8.39	1.58	1.46
1	F	305	GLY	N-CA	6.06	1.55	1.46
1	D	305	GLY	C-N	5.81	1.43	1.33
1	D	406	GLY	N-CA	5.52	1.54	1.46
1	D	405	SER	CA-CB	5.39	1.61	1.52
1	F	406	GLY	C-N	5.14	1.42	1.33
1	E	406	GLY	CA-C	-5.04	1.43	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	454	PHE	Peptide

## 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	1265	0	1217	23	0
1	B	1280	0	1224	18	0
1	C	1292	0	1243	18	0
1	D	1299	0	1243	28	0
1	E	1273	0	1227	21	0
1	F	1269	0	1211	23	0
2	A	1	0	0	0	0
3	B	6	0	8	5	0
4	A	215	0	0	5	0
4	B	184	0	0	4	0
4	C	193	0	0	4	0
4	D	203	0	0	9	0
4	E	195	0	0	5	0
4	F	176	0	0	3	0
All	All	8851	0	7373	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 8.

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:C:430:VAL:HG23	4:C:478:HOH:O	1.52	1.09
1:E:389:ASN:HB3	4:E:549:HOH:O	1.73	0.86
1:F:337:VAL:CG2	1:F:353:PRO:HD2	2.13	0.79
1:D:389[A]:ASN:HB2	4:D:626:HOH:O	1.84	0.78
1:A:337[A]:VAL:CG2	1:A:353:PRO:HD2	2.14	0.78
1:C:338:ASN:HB3	4:E:477:HOH:O	1.84	0.77
1:F:337:VAL:HG21	1:F:353:PRO:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:VAL:HB	4:D:602:HOH:O	1.83	0.76
1:A:455:THR:OXT	1:A:455:THR:HG22	1.83	0.76
1:E:415:ASN:HD21	1:F:445:ALA:H	1.34	0.75
1:D:421:TRP:CD1	4:D:468:HOH:O	2.43	0.72
1:A:418:VAL:HG13	4:A:2062:HOH:O	1.89	0.71
1:D:303:VAL:HG23	1:D:304:SER:H	1.56	0.71
1:D:452:ARG:HD3	4:D:493:HOH:O	1.92	0.69
1:B:452:ARG:NH2	4:B:2543:HOH:O	2.25	0.69
1:F:319:MET:HB3	1:F:375:LEU:HD22	1.75	0.69
1:A:337[A]:VAL:HG21	1:A:353:PRO:HD2	1.75	0.68
1:F:427:ARG:NH1	4:F:551:HOH:O	2.27	0.68
1:B:427:ARG:HG3	4:B:2519:HOH:O	1.95	0.67
1:C:416:LEU:HD12	1:C:430:VAL:HG22	1.79	0.65
1:A:445:ALA:H	1:C:415:ASN:HD21	1.44	0.64
1:C:370:PHE:HB2	4:C:504:HOH:O	1.98	0.64
1:A:455:THR:OXT	1:A:455:THR:CG2	2.45	0.63
1:D:349:HIS:HD2	1:D:449:SER:OG	1.81	0.63
1:D:319:MET:HE2	1:D:321:ILE:HD11	1.80	0.63
1:E:415:ASN:HD21	1:F:445:ALA:N	1.96	0.63
1:D:426:LEU:HD13	4:D:468:HOH:O	1.99	0.62
1:D:427[A]:ARG:NH1	4:D:525:HOH:O	2.34	0.61
1:F:372:THR:HG23	4:F:490:HOH:O	2.00	0.60
1:A:337[A]:VAL:CG2	1:A:353:PRO:CD	2.80	0.60
1:C:324:VAL:HG22	1:C:368:LEU:HD22	1.82	0.59
1:F:294:PRO:HA	4:F:519:HOH:O	2.02	0.59
1:E:417:TRP:CZ2	1:E:429:ARG:HG2	2.38	0.59
1:E:415:ASN:ND2	1:F:445:ALA:H	2.01	0.58
1:F:362[A]:ASP:OD1	1:F:435:SER:HB2	2.03	0.58
1:F:337:VAL:CG2	1:F:353:PRO:CD	2.81	0.58
1:F:303:VAL:N	1:F:306:GLY:O	2.28	0.57
1:A:445:ALA:N	1:C:415:ASN:HD21	2.02	0.57
1:B:415:ASN:HD21	1:C:445:ALA:H	1.52	0.57
3:B:2500:GOL:C1	1:E:332:ASN:HD22	2.19	0.56
1:D:445:ALA:H	1:F:415:ASN:HD21	1.54	0.54
1:E:334:ARG:NH2	4:E:477:HOH:O	2.41	0.53
1:A:415:ASN:HD21	1:B:445:ALA:H	1.55	0.53
1:D:374:LEU:HD13	1:D:378:LEU:HD22	1.90	0.53
1:D:349:HIS:HE1	1:F:347:TYR:OH	1.92	0.53
1:B:415:ASN:HD21	1:C:445:ALA:N	2.08	0.52
1:B:416:LEU:HD12	1:B:430:VAL:HG22	1.92	0.52
1:D:445:ALA:N	1:F:415:ASN:HD21	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:MET:CE	1:D:321:ILE:HD11	2.40	0.52
1:D:415:ASN:HD21	1:E:445:ALA:H	1.58	0.52
1:B:324:VAL:HG22	1:B:368:LEU:HD22	1.91	0.51
1:C:337[A]:VAL:HG22	1:C:353:PRO:HG2	1.92	0.50
1:D:421:TRP:HD1	4:D:468:HOH:O	1.89	0.50
1:C:337[A]:VAL:HG22	1:C:353:PRO:CG	2.43	0.49
1:A:415:ASN:HD21	1:B:445:ALA:N	2.10	0.49
1:A:394:TYR:CZ	1:A:451:PRO:HD3	2.47	0.49
1:E:416:LEU:HD12	1:E:430:VAL:HG22	1.95	0.49
1:C:421:TRP:CZ2	1:C:424:GLY:HA2	2.48	0.48
3:B:2500:GOL:H11	1:E:332:ASN:ND2	2.29	0.48
1:E:427[A]:ARG:NH1	4:E:551:HOH:O	2.47	0.47
3:B:2500:GOL:H11	1:E:332:ASN:HD22	1.79	0.47
1:A:418:VAL:CG1	4:A:2062:HOH:O	2.56	0.47
1:E:324:VAL:HG22	1:E:368[A]:LEU:HD23	1.95	0.47
1:C:341[B]:ILE:CD1	1:C:350:ILE:HG23	2.45	0.47
1:F:337:VAL:HG23	1:F:353:PRO:HG2	1.96	0.47
1:A:442:LYS:HE3	4:A:2172:HOH:O	2.14	0.46
1:E:379:LEU:O	1:E:382:ASP:HB2	2.16	0.46
1:D:403:LEU:CD1	1:D:412:MET:HG3	2.46	0.46
1:F:413:SER:O	1:F:433:GLY:HA3	2.16	0.46
1:C:366:LEU:N	4:C:478:HOH:O	2.48	0.46
1:A:321:ILE:HG23	1:A:338:ASN:OD1	2.16	0.45
3:B:2500:GOL:H31	1:E:330:GLY:HA2	1.98	0.45
1:F:337:VAL:HG23	1:F:353:PRO:CG	2.46	0.45
1:A:445:ALA:H	1:C:415:ASN:ND2	2.14	0.45
1:F:416:LEU:HD12	1:F:430:VAL:HG22	1.97	0.45
1:D:403:LEU:HD12	1:D:412:MET:HG3	1.99	0.45
1:A:454:PHE:O	1:A:455:THR:HB	2.17	0.44
1:C:389:ASN:ND2	4:C:606:HOH:O	2.36	0.44
1:D:374:LEU:HD13	1:D:378:LEU:CD2	2.47	0.44
1:B:335[A]:VAL:HG12	1:B:336:GLN:N	2.33	0.44
1:A:451:PRO:HG3	1:B:344:VAL:HG21	1.99	0.43
1:D:394:TYR:CZ	1:D:451:PRO:HD3	2.53	0.43
1:E:416:LEU:HA	1:E:429:ARG:O	2.18	0.43
1:A:337[A]:VAL:HG22	1:A:353:PRO:CD	2.49	0.43
1:F:320:TRP:HB2	1:F:341:ILE:HD11	2.01	0.43
1:D:349:HIS:CE1	1:F:347:TYR:OH	2.70	0.43
1:C:384:GLU:HA	1:C:385:PRO:HD3	1.92	0.43
1:B:408:THR:HA	1:B:409:PRO:HD3	1.88	0.43
1:B:435:SER:OG	1:B:436:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ASN:HD21	1:E:445:ALA:N	2.15	0.43
1:E:353:PRO:HG2	4:E:542:HOH:O	2.18	0.43
1:A:324:VAL:HG22	1:A:368:LEU:HD22	2.01	0.43
1:A:385:PRO:HD3	1:A:421:TRP:CG	2.54	0.42
1:B:416:LEU:HA	1:B:429:ARG:O	2.18	0.42
1:B:421:TRP:CZ2	1:B:424:GLY:HA2	2.54	0.42
1:D:349:HIS:CD2	1:D:449:SER:OG	2.67	0.42
1:B:366:LEU:HD13	1:B:443:TRP:CH2	2.55	0.42
1:B:437:THR:HA	4:B:2549:HOH:O	2.18	0.42
1:B:327:SER:HA	1:B:331:LEU:O	2.20	0.42
1:C:341[B]:ILE:HD11	1:C:350:ILE:HG23	2.01	0.42
1:D:421:TRP:CZ2	1:D:424:GLY:HA2	2.56	0.41
1:D:303:VAL:HG23	1:D:304:SER:N	2.31	0.41
1:B:365:ASP:HB3	4:B:2519:HOH:O	2.19	0.41
1:D:442:LYS:HE2	4:D:480:HOH:O	2.20	0.41
1:E:324:VAL:HG22	1:E:368[A]:LEU:CD2	2.50	0.41
1:F:439:SER:OG	1:F:440:ASN:ND2	2.54	0.41
1:A:354:ALA:HA	4:A:2110:HOH:O	2.21	0.40
1:D:316[A]:ARG:HD2	1:D:343:ILE:HD12	2.03	0.40
3:B:2500:GOL:C2	1:E:330:GLY:O	2.70	0.40
1:A:416:LEU:HA	1:A:429:ARG:O	2.21	0.40
1:E:384:GLU:HA	1:E:385:PRO:HD3	1.91	0.40
1:A:359:SER:HB3	4:A:2174:HOH:O	2.22	0.40
1:D:420:GLN:NE2	4:D:626:HOH:O	2.55	0.40
1:F:333:TRP:CD1	1:F:358:PHE:HB2	2.57	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	163/165 (99%)	157 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	165/165 (100%)	160 (97%)	5 (3%)	0	100	100
1	C	166/165 (101%)	158 (95%)	8 (5%)	0	100	100
1	D	166/165 (101%)	159 (96%)	7 (4%)	0	100	100
1	E	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
1	F	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
All	All	986/990 (100%)	949 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	139/138 (101%)	133 (96%)	6 (4%)	29	9
1	B	141/138 (102%)	141 (100%)	0	100	100
1	C	142/138 (103%)	140 (99%)	2 (1%)	67	52
1	D	142/138 (103%)	140 (99%)	2 (1%)	67	52
1	E	139/138 (101%)	138 (99%)	1 (1%)	84	75
1	F	139/138 (101%)	137 (99%)	2 (1%)	67	52
All	All	842/828 (102%)	829 (98%)	13 (2%)	65	49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	THR
1	A	375	LEU
1	A	422	GLN
1	A	435	SER
1	A	449	SER
1	A	455	THR
1	C	337[A]	VAL
1	C	337[B]	VAL

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Mol	Chain	Res	Type
1	D	334	ARG
1	D	435	SER
1	E	365	ASP
1	F	375	LEU
1	F	378	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	A	440	ASN
1	B	410	GLN
1	B	415	ASN
1	B	440	ASN
1	C	410	GLN
1	C	415	ASN
1	C	440	ASN
1	D	317	GLN
1	D	349	HIS
1	D	415	ASN
1	D	440	ASN
1	E	312	ASN
1	E	336	GLN
1	E	415	ASN
1	E	440	ASN
1	F	338	ASN
1	F	388	HIS
1	F	410	GLN
1	F	415	ASN
1	F	440	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	B	2500	-	5,5,5	0.34	0	5,5,5	0.37	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	B	2500	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2500	GOL	C1-C2-C3-O3
3	B	2500	GOL	O2-C2-C3-O3
3	B	2500	GOL	O1-C1-C2-C3
3	B	2500	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2500	GOL	5	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, 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	162/165 (98%)	0.64	6 (3%) 41 48	8, 13, 21, 26	0
1	B	163/165 (98%)	0.68	8 (4%) 29 35	7, 13, 22, 34	0
1	C	162/165 (98%)	0.61	8 (4%) 29 35	8, 13, 22, 29	0
1	D	160/165 (96%)	0.92	22 (13%) 2 4	9, 13, 27, 37	0
1	E	161/165 (97%)	0.67	10 (6%) 20 26	7, 13, 23, 32	0
1	F	163/165 (98%)	0.94	17 (10%) 6 9	9, 14, 26, 36	1 (0%)
All	All	971/990 (98%)	0.74	71 (7%) 15 20	7, 13, 24, 37	1 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	406	GLY	6.9
1	A	455	THR	6.3
1	D	305	GLY	6.2
1	E	305	GLY	5.9
1	F	293	SER	5.7
1	D	406	GLY	5.6
1	B	455	THR	5.3
1	D	306	GLY	5.1
1	F	294	PRO	5.1
1	D	295	ASN	4.7
1	D	303	VAL	4.6
1	F	306	GLY	4.6
1	B	436	ILE	4.4
1	F	455	THR	4.2
1	D	407	GLY	4.1
1	F	407	GLY	4.0
1	C	407	GLY	3.9
1	E	306	GLY	3.8
1	D	296	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	304	SER	3.7
1	A	406	GLY	3.7
1	F	406	GLY	3.7
1	E	294	PRO	3.6
1	B	293	SER	3.6
1	E	304	SER	3.5
1	C	293	SER	3.4
1	C	294	PRO	3.4
1	E	308	GLY	3.3
1	D	304	SER	3.2
1	F	305	GLY	3.2
1	E	295	ASN	3.1
1	F	296	LEU	3.1
1	F	304	SER	3.0
1	F	408	THR	3.0
1	F	377	PRO	2.9
1	D	378	LEU	2.8
1	D	434	GLY	2.8
1	D	381	GLY	2.7
1	A	305	GLY	2.7
1	B	437	THR	2.7
1	B	408	THR	2.7
1	B	294	PRO	2.6
1	F	301	ALA	2.6
1	D	437	THR	2.6
1	D	435	SER	2.5
1	D	448	VAL	2.5
1	F	312	ASN	2.4
1	B	335[A]	VAL	2.4
1	E	307	ILE	2.4
1	F	302	ASP	2.4
1	E	407	GLY	2.4
1	D	307[A]	ILE	2.4
1	F	405	SER	2.3
1	F	375	LEU	2.3
1	A	294	PRO	2.3
1	D	308	GLY	2.3
1	F	307	ILE	2.2
1	C	435	SER	2.2
1	C	305	GLY	2.2
1	D	377	PRO	2.2
1	D	408	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	358	PHE	2.2
1	D	302	ASP	2.2
1	B	435	SER	2.1
1	C	302	ASP	2.1
1	E	434	GLY	2.1
1	C	358	PHE	2.1
1	C	408	THR	2.1
1	D	436	ILE	2.1
1	A	337[A]	VAL	2.0
1	D	309	MET	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	2500	6/6	0.79	0.19	22,23,24,25	0
2	MG	A	2001	1/1	0.92	0.08	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.