



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 02:13 pm GMT

PDB ID : 4CC7  
Title : Crystal structure of the sixth or C-terminal SH3 domain of human Tuba in complex with proline-rich peptides of N-WASP. Space group P41  
Authors : Polle, L.; Rigano, L.; Julian, R.; Ireton, K.; Schubert, W.-D.  
Deposited on : 2013-10-18  
Resolution : 1.97 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.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

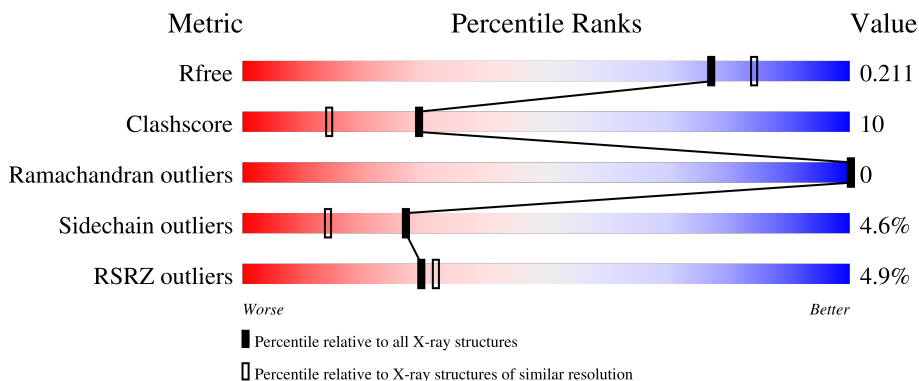
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	67	
1	C	67	
1	E	67	
1	G	67	
1	I	67	

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Mol	Chain	Length	Quality of chain
1	K	67	<p>4% 67% 18% 6% 9%</p>
1	M	67	<p>4% 66% 21% 10%</p>
2	B	12	<p>8% 83% 8% 8%</p>
2	D	12	<p>8% 67% 25% 8%</p>
2	F	12	<p>8% 67% 33%</p>
2	H	12	<p>8% 83% 17%</p>
2	J	12	<p>8% 92% 8%</p>
2	L	12	<p>8% 92% 8%</p>
2	N	12	<p>8% 92% 8%</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4418 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 DYNAMIN-BINDING PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	59	521	340	91	90	0	10	1
1	C	63	529	343	89	97	0	2	0
1	E	62	546	354	94	98	0	7	0
1	G	61	505	330	84	91	0	1	0
1	I	61	515	333	89	93	0	2	0
1	K	61	534	350	91	93	0	10	1
1	M	60	502	330	84	88	0	4	1

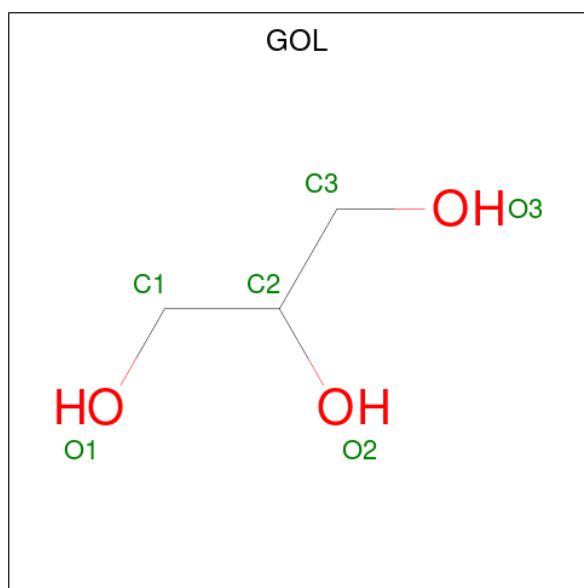
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1511	GLY	-	expression tag	UNP Q6XZF7
A	1512	PRO	-	expression tag	UNP Q6XZF7
C	1511	GLY	-	expression tag	UNP Q6XZF7
C	1512	PRO	-	expression tag	UNP Q6XZF7
E	1511	GLY	-	expression tag	UNP Q6XZF7
E	1512	PRO	-	expression tag	UNP Q6XZF7
G	1511	GLY	-	expression tag	UNP Q6XZF7
G	1512	PRO	-	expression tag	UNP Q6XZF7
I	1511	GLY	-	expression tag	UNP Q6XZF7
I	1512	PRO	-	expression tag	UNP Q6XZF7
K	1511	GLY	-	expression tag	UNP Q6XZF7
K	1512	PRO	-	expression tag	UNP Q6XZF7
M	1511	GLY	-	expression tag	UNP Q6XZF7
M	1512	PRO	-	expression tag	UNP Q6XZF7

- Molecule 2 is a protein called NEURAL WISKOTT-ALDRICH SYNDROME PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	1	1
			68	44	11	13			
2	D	12	Total	C	N	O	0	0	1
			73	47	12	14			
2	F	12	Total	C	N	O	0	0	1
			73	47	12	14			
2	H	12	Total	C	N	O	0	0	0
			75	48	12	15			
2	J	12	Total	C	N	O	0	0	1
			72	46	12	14			
2	L	12	Total	C	N	O	0	0	1
			68	43	11	14			
2	N	12	Total	C	N	O	0	0	1
			73	47	12	14			

- 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	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	C	3	Total Cl 3 3	0	0
4	E	2	Total Cl 2 2	0	0
4	G	2	Total Cl 2 2	0	0
4	I	1	Total Cl 1 1	0	0
4	K	3	Total Cl 3 3	0	0
4	M	4	Total Cl 4 4	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total Mg 1 1	0	0
5	M	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	20	Total O 20 20	0	0
6	C	44	Total O 44 44	0	0
6	D	1	Total O 1 1	0	0
6	E	29	Total O 29 29	0	0
6	F	4	Total O 4 4	0	0
6	G	30	Total O 30 30	0	0
6	H	1	Total O 1 1	0	0
6	I	21	Total O 21 21	0	0

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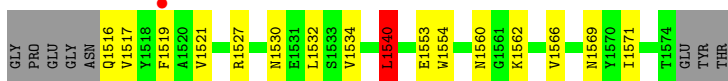
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	K	31	Total 31	O 31	0	0
6	L	4	Total 4	O 4	0	0
6	M	31	Total 31	O 31	0	0
6	N	5	Total 5	O 5	0	0

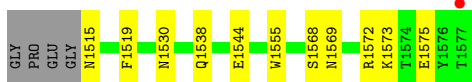
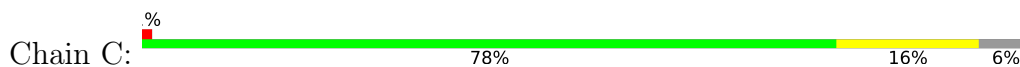
### 3 Residue-property plots [i](#)

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.

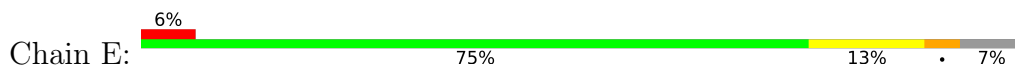
- Molecule 1: DYNAMIN-BINDING PROTEIN



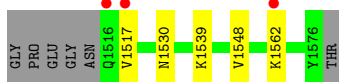
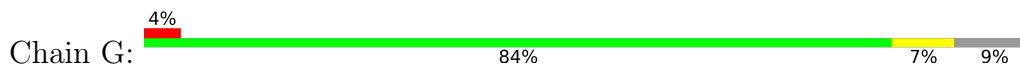
- Molecule 1: DYNAMIN-BINDING PROTEIN



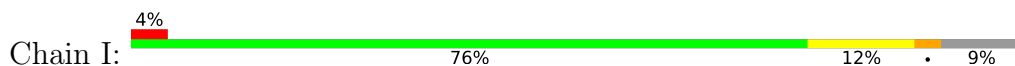
- Molecule 1: DYNAMIN-BINDING PROTEIN



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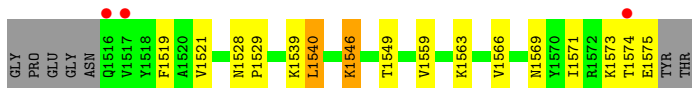


- Molecule 1: DYNAMIN-BINDING PROTEIN

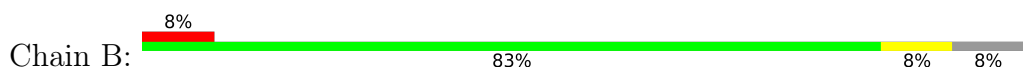




- Molecule 1: DYNAMIN-BINDING PROTEIN



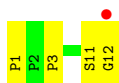
- Molecule 2: NEURAL WISKOTT-ALDRICH SYNDROME PROTEIN



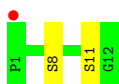
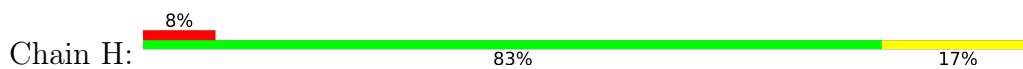
- Molecule 2: NEURAL WISKOTT-ALDRICH SYNDROME PROTEIN



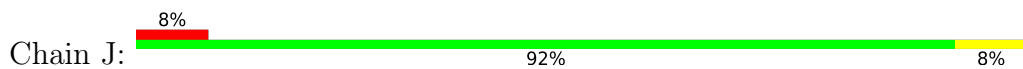
- Molecule 2: NEURAL WISKOTT-ALDRICH SYNDROME PROTEIN



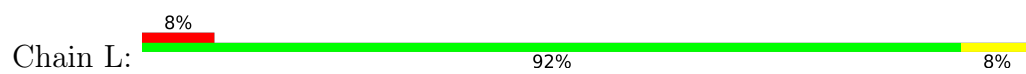
- Molecule 2: NEURAL WISKOTT-ALDRICH SYNDROME PROTEIN



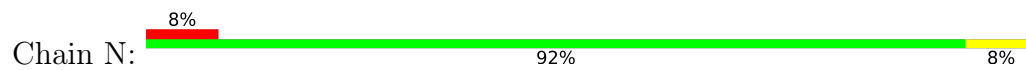
- Molecule 2: NEURAL WISKOTT-ALDRICH SYNDROME PROTEIN



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- Molecule 2: NEURAL WISKOTT-ALDRICH SYNDROME PROTEIN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.57Å 88.57Å 69.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.59 – 1.97 44.28 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.59-1.97) 99.8 (44.28-1.97)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.176 , 0.215 0.177 , 0.211	Depositor DCC
$R_{free}$ test set	1920 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtrriage
Anisotropy	0.284	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, 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	0.94	0/579	1.06	1/780 (0.1%)
1	C	1.10	1/553 (0.2%)	1.03	0/747
1	E	0.88	0/585	0.92	0/789
1	G	0.91	0/523	0.89	0/707
1	I	0.95	1/535 (0.2%)	1.08	7/722 (1.0%)
1	K	1.18	0/589	1.06	2/798 (0.3%)
1	M	0.96	0/531	0.98	1/719 (0.1%)
2	B	0.80	0/76	0.73	0/107
2	D	1.44	1/77 (1.3%)	0.82	0/108
2	F	1.14	1/77 (1.3%)	1.02	0/108
2	H	0.83	0/79	0.69	0/110
2	J	0.70	0/76	0.71	0/107
2	L	0.96	0/71	0.71	0/100
2	N	1.00	0/77	0.79	0/108
All	All	1.00	4/4428 (0.1%)	0.98	11/6010 (0.2%)

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	K	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	12	GLY	N-CA	9.86	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1518	TYR	CE2-CZ	-8.23	1.27	1.38
1	C	1544	GLU	CD-OE2	-6.68	1.18	1.25
2	F	12	GLY	N-CA	5.84	1.54	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	LEU	CB-CG-CD1	-13.13	88.67	111.00
1	I	1518	TYR	OH-CZ-CE2	-6.97	101.27	120.10
1	I	1572[A]	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	I	1572[B]	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	I	1518	TYR	CE1-CZ-OH	6.58	137.87	120.10
1	I	1572[A]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	I	1572[B]	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	K	1572	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	K	1527	ARG	CG-CD-NE	5.38	123.10	111.80
1	I	1530	ASN	CB-CA-C	-5.24	99.93	110.40
1	M	1546	LYS	CB-CG-CD	5.02	124.66	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	11	SER	Peptide
2	F	11	SER	Peptide
1	K	1515	ASN	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	521	0	537	13	0
1	C	529	0	527	5	0
1	E	546	0	548	15	0
1	G	505	0	502	2	0
1	I	515	0	519	7	0
1	K	534	0	562	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	502	0	517	11	0
2	B	68	0	71	1	0
2	D	73	0	74	2	0
2	F	73	0	74	2	0
2	H	75	0	76	1	0
2	J	72	0	73	1	0
2	L	68	0	64	1	0
2	N	73	0	74	1	0
3	A	6	0	8	0	0
3	C	6	0	8	3	0
3	K	6	0	8	1	0
3	M	6	0	8	0	0
4	A	2	0	0	0	0
4	C	3	0	0	0	0
4	E	2	0	0	1	0
4	G	2	0	0	0	0
4	I	1	0	0	0	0
4	K	3	0	0	0	0
4	M	4	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
6	A	20	0	0	3	0
6	C	44	0	0	2	0
6	D	1	0	0	1	0
6	E	29	0	0	0	0
6	F	4	0	0	1	0
6	G	30	0	0	0	0
6	H	1	0	0	0	0
6	I	21	0	0	2	0
6	K	31	0	0	2	0
6	L	4	0	0	0	0
6	M	31	0	0	1	0
6	N	5	0	0	0	0
All	All	4418	0	4250	82	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 10.

All (82) 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:1527[A]:ARG:NH2	6:A:2002:HOH:O	1.78	1.15
1:A:1519:PHE:CE2	1:A:1521:VAL:HG12	1.88	1.08
1:K:1566[B]:VAL:HG23	1:K:1571[B]:ILE:HD11	1.47	0.96
1:K:1566[B]:VAL:CG2	1:K:1571[B]:ILE:HD11	1.99	0.91
1:E:1515[B]:ASN:O	1:E:1516[B]:GLN:HB2	1.71	0.90
1:E:1532:LEU:HD21	1:E:1559[B]:VAL:HG13	1.65	0.78
2:D:12:GLY:CA	2:L:12:GLY:N	2.50	0.74
1:K:1515:ASN:HB3	1:K:1545:PHE:HZ	1.54	0.73
1:K:1515:ASN:HB3	1:K:1545:PHE:CZ	2.28	0.69
1:A:1519:PHE:HE2	1:A:1521:VAL:HG12	1.54	0.66
1:E:1528:ASN:HD22	1:E:1530:ASN:H	1.45	0.65
1:E:1515[A]:ASN:ND2	1:E:1516[A]:GLN:H	1.97	0.63
1:A:1519:PHE:CE2	1:A:1521:VAL:CG1	2.74	0.62
3:C:2578:GOL:C3	6:C:2044:HOH:O	2.47	0.62
1:E:1515[A]:ASN:CG	1:E:1516[A]:GLN:N	2.53	0.61
1:K:1566[B]:VAL:HG21	1:K:1571[B]:ILE:HD11	1.80	0.61
1:E:1528:ASN:ND2	1:E:1529:PRO:HD2	2.18	0.59
1:M:1575:GLU:N	6:M:2031:HOH:O	2.36	0.59
1:E:1515[A]:ASN:CG	1:E:1516[A]:GLN:H	2.05	0.59
1:A:1560:ASN:OD1	6:A:2016:HOH:O	2.16	0.58
1:K:1573[B]:LYS:HD3	1:K:1574:THR:N	2.20	0.56
1:K:1528[A]:ASN:HD21	1:K:1530:ASN:ND2	2.04	0.56
2:F:1:PRO:HD2	6:F:2001:HOH:O	2.05	0.56
1:M:1573:LYS:HD3	1:M:1574:THR:N	2.21	0.55
1:E:1516[B]:GLN:HE22	1:E:1541:LYS:HE2	1.72	0.55
1:K:1566[A]:VAL:HG11	1:K:1571[A]:ILE:HD11	1.88	0.55
1:M:1519:PHE:CE2	1:M:1521:VAL:HG22	2.42	0.54
1:E:1515[A]:ASN:OD1	1:E:1573:LYS:NZ	2.40	0.54
1:A:1553:GLU:OE1	6:A:2013:HOH:O	2.19	0.54
1:E:1515[A]:ASN:O	1:E:1516[A]:GLN:HB2	2.08	0.53
1:A:1566[B]:VAL:HG11	1:A:1571:ILE:HD11	1.90	0.53
1:C:1515:ASN:OD1	1:C:1573:LYS:NZ	2.41	0.52
1:M:1549:THR:HG23	2:N:11:SER:OG	2.11	0.50
6:D:2001:HOH:O	1:K:1528[A]:ASN:ND2	2.44	0.50
1:E:1562[B]:LYS:NZ	4:E:2578:CL:CL	2.82	0.50
1:K:1539:LYS:HD2	1:K:1539:LYS:N	2.26	0.50
1:M:1540[B]:LEU:HD22	1:M:1559:VAL:CG2	2.42	0.50
1:I:1548:VAL:HG22	2:J:11:SER:O	2.12	0.48
1:C:1519:PHE:CD2	1:C:1575:GLU:OE2	2.66	0.48
1:E:1516[B]:GLN:NE2	1:E:1541:LYS:HE2	2.27	0.47
1:E:1532:LEU:HD11	1:E:1562[B]:LYS:HG3	1.96	0.47
1:I:1571:ILE:O	1:I:1572[A]:ARG:NE	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1515:ASN:N	6:I:2002:HOH:O	2.47	0.47
1:K:1516[A]:GLN:HG2	1:K:1573[A]:LYS:NZ	2.30	0.47
1:A:1516:GLN:HB3	1:A:1517:VAL:H	1.55	0.46
1:M:1539[A]:LYS:HE3	1:M:1574:THR:HG22	1.98	0.46
3:C:2578:GOL:H32	6:C:2044:HOH:O	2.11	0.45
1:I:1518:TYR:OH	1:I:1573:LYS:HE2	2.16	0.45
1:K:1528[A]:ASN:ND2	6:K:2009:HOH:O	2.48	0.45
1:K:1540[A]:LEU:CD1	1:K:1571[A]:ILE:HD12	2.47	0.44
1:G:1548:VAL:HG22	2:H:11:SER:O	2.18	0.44
1:K:1516[A]:GLN:CG	1:K:1573[A]:LYS:NZ	2.81	0.44
1:C:1555:TRP:CD1	1:C:1568:SER:HB3	2.53	0.44
1:C:1572:ARG:HD2	3:C:2578:GOL:H2	1.99	0.43
1:K:1573[B]:LYS:HD3	1:K:1574:THR:H	1.82	0.43
1:I:1517:VAL:HG11	1:I:1539:LYS:HE2	2.01	0.43
1:I:1515:ASN:CB	6:I:2002:HOH:O	2.67	0.43
1:K:1569[B]:ASN:ND2	6:K:2024:HOH:O	2.45	0.43
1:E:1521:VAL:HG23	1:E:1522:TYR:CD2	2.54	0.43
1:K:1519:PHE:HB3	1:K:1539:LYS:HE3	2.01	0.42
1:M:1539[A]:LYS:HE3	1:M:1574:THR:CG2	2.49	0.42
1:C:1519:PHE:CD2	1:C:1575:GLU:CD	2.92	0.42
1:A:1554:TRP:CG	2:B:10:PRO:HB3	2.55	0.42
1:M:1566:VAL:HG11	1:M:1571[B]:ILE:HD11	2.00	0.42
1:I:1571:ILE:O	1:I:1572[B]:ARG:HD3	2.20	0.41
2:D:1:PRO:N	2:D:2:PRO:CD	2.83	0.41
1:E:1522:TYR:CE2	2:F:3:PRO:HD3	2.56	0.41
1:K:1528[A]:ASN:ND2	1:K:1530:ASN:ND2	2.67	0.41
1:K:1566[B]:VAL:HG23	1:K:1571[B]:ILE:CD1	2.35	0.41
1:A:1534:VAL:HG11	1:A:1540:LEU:HD23	2.02	0.41
1:G:1517:VAL:HG11	1:G:1539:LYS:HE2	2.02	0.40
1:K:1535:SER:OG	3:K:2576:GOL:H12	2.20	0.40
1:M:1528:ASN:HB2	1:M:1529:PRO:CD	2.52	0.40
1:K:1566[A]:VAL:CG1	1:K:1571[A]:ILE:HD11	2.50	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	67/67 (100%)	67 (100%)	0	0	100	100
1	C	63/67 (94%)	63 (100%)	0	0	100	100
1	E	66/67 (98%)	64 (97%)	2 (3%)	0	100	100
1	G	60/67 (90%)	60 (100%)	0	0	100	100
1	I	61/67 (91%)	61 (100%)	0	0	100	100
1	K	69/67 (103%)	67 (97%)	2 (3%)	0	100	100
1	M	62/67 (92%)	62 (100%)	0	0	100	100
2	B	10/12 (83%)	10 (100%)	0	0	100	100
2	D	10/12 (83%)	10 (100%)	0	0	100	100
2	F	10/12 (83%)	10 (100%)	0	0	100	100
2	H	10/12 (83%)	10 (100%)	0	0	100	100
2	J	10/12 (83%)	10 (100%)	0	0	100	100
2	L	10/12 (83%)	10 (100%)	0	0	100	100
2	N	10/12 (83%)	10 (100%)	0	0	100	100
All	All	518/553 (94%)	514 (99%)	4 (1%)	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	61/58 (105%)	57 (93%)	4 (7%)	16	7
1	C	58/58 (100%)	55 (95%)	3 (5%)	23	11
1	E	62/58 (107%)	57 (92%)	5 (8%)	11	3
1	G	54/58 (93%)	51 (94%)	3 (6%)	21	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	56/58 (97%)	55 (98%)	1 (2%)	59	51
1	K	63/58 (109%)	59 (94%)	4 (6%)	18	7
1	M	56/58 (97%)	51 (91%)	5 (9%)	9	2
2	B	9/9 (100%)	9 (100%)	0	100	100
2	D	9/9 (100%)	9 (100%)	0	100	100
2	F	9/9 (100%)	9 (100%)	0	100	100
2	H	9/9 (100%)	8 (89%)	1 (11%)	6	1
2	J	9/9 (100%)	9 (100%)	0	100	100
2	L	8/9 (89%)	8 (100%)	0	100	100
2	N	9/9 (100%)	9 (100%)	0	100	100
All	All	472/469 (101%)	446 (94%)	26 (6%)	27	10

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1530	ASN
1	A	1540	LEU
1	A	1569[A]	ASN
1	A	1569[B]	ASN
1	C	1530	ASN
1	C	1538	GLN
1	C	1569	ASN
1	E	1515[A]	ASN
1	E	1515[B]	ASN
1	E	1528	ASN
1	E	1562[A]	LYS
1	E	1562[B]	LYS
1	G	1530	ASN
1	G	1562[A]	LYS
1	G	1562[B]	LYS
2	H	8	SER
1	I	1546	LYS
1	K	1516[A]	GLN
1	K	1516[B]	GLN
1	K	1530	ASN
1	K	1574	THR
1	M	1540[A]	LEU
1	M	1540[B]	LEU

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Mol	Chain	Res	Type
1	M	1546	LYS
1	M	1563	LYS
1	M	1569	ASN

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

Mol	Chain	Res	Type
1	A	1530	ASN
1	C	1560	ASN
1	C	1569	ASN
1	E	1528	ASN
1	G	1528	ASN
1	G	1530	ASN
1	G	1560	ASN
1	I	1560	ASN
1	K	1530	ASN
1	M	1569	ASN

### 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 23 ligands modelled in this entry, 19 are monoatomic - leaving 4 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	K	2576	-	5,5,5	0.57	0	5,5,5	0.50	0
3	GOL	M	2576	-	5,5,5	0.45	0	5,5,5	0.48	0
3	GOL	C	2578	-	5,5,5	0.60	0	5,5,5	1.12	1 (20%)
3	GOL	A	2575	-	5,5,5	0.60	0	5,5,5	2.05	2 (40%)

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	K	2576	-	-	4/4/4/4	-
3	GOL	M	2576	-	-	2/4/4/4	-
3	GOL	C	2578	-	-	4/4/4/4	-
3	GOL	A	2575	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2575	GOL	O3-C3-C2	-3.75	92.23	110.20
3	A	2575	GOL	O2-C2-C1	2.24	118.97	109.12
3	C	2578	GOL	O3-C3-C2	2.13	120.40	110.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2578	GOL	C1-C2-C3-O3
3	C	2578	GOL	O2-C2-C3-O3
3	K	2576	GOL	O1-C1-C2-C3
3	K	2576	GOL	C1-C2-C3-O3
3	M	2576	GOL	O1-C1-C2-C3
3	A	2575	GOL	O2-C2-C3-O3
3	C	2578	GOL	O1-C1-C2-O2
3	A	2575	GOL	C1-C2-C3-O3
3	C	2578	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	K	2576	GOL	O1-C1-C2-O2
3	K	2576	GOL	O2-C2-C3-O3
3	M	2576	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	2576	GOL	1	0
3	C	2578	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	59/67 (88%)	0.53	1 (1%) 70 71	24, 44, 67, 75	0
1	C	63/67 (94%)	0.28	1 (1%) 72 73	23, 32, 53, 71	0
1	E	62/67 (92%)	0.40	4 (6%) 18 20	26, 38, 58, 73	0
1	G	61/67 (91%)	0.32	3 (4%) 29 32	30, 39, 58, 69	0
1	I	61/67 (91%)	0.49	3 (4%) 29 32	32, 44, 69, 79	0
1	K	61/67 (91%)	0.56	3 (4%) 29 32	22, 32, 59, 82	0
1	M	60/67 (89%)	0.39	3 (5%) 28 31	27, 36, 62, 71	0
2	B	11/12 (91%)	0.61	1 (9%) 9 10	36, 47, 75, 88	0
2	D	12/12 (100%)	0.45	1 (8%) 11 12	29, 39, 58, 76	0
2	F	12/12 (100%)	0.45	1 (8%) 11 12	34, 42, 46, 61	0
2	H	12/12 (100%)	0.68	1 (8%) 11 12	41, 49, 68, 69	0
2	J	12/12 (100%)	0.97	1 (8%) 11 12	47, 60, 77, 79	0
2	L	12/12 (100%)	0.37	1 (8%) 11 12	29, 39, 68, 83	0
2	N	12/12 (100%)	0.53	1 (8%) 11 12	36, 47, 66, 82	0
All	All	510/553 (92%)	0.45	25 (4%) 29 32	22, 39, 68, 88	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	1515	ASN	6.5
1	M	1517[A]	VAL	5.3
1	K	1574	THR	4.5
1	M	1574	THR	4.3
2	J	1	PRO	4.1
1	E	1516[A]	GLN	3.5
2	N	1	PRO	3.3
1	E	1517	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	1517[A]	VAL	3.2
2	H	1	PRO	2.9
1	A	1519	PHE	2.9
1	G	1517	VAL	2.7
1	E	1515[A]	ASN	2.7
2	L	1	PRO	2.6
1	I	1519	PHE	2.6
1	I	1515	ASN	2.5
1	C	1577	THR	2.4
1	G	1562[A]	LYS	2.4
1	M	1516	GLN	2.4
2	D	1	PRO	2.4
2	B	2	PRO	2.3
1	E	1576	TYR	2.3
1	G	1516	GLN	2.2
2	F	12	GLY	2.2
1	I	1575	GLU	2.1

## 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	K	2576	6/6	0.70	0.30	43,66,76,81	0
5	MG	M	2577	1/1	0.72	0.12	53,53,53,53	0
3	GOL	A	2575	6/6	0.84	0.20	38,55,62,64	0
4	CL	C	2581	1/1	0.88	0.14	47,47,47,47	1
4	CL	E	2578	1/1	0.89	0.24	49,49,49,49	1
4	CL	M	2580	1/1	0.91	0.12	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	C	2578	6/6	0.92	0.31	33,58,60,62	0
3	GOL	M	2576	6/6	0.92	0.15	33,54,59,62	0
4	CL	I	2576	1/1	0.93	0.12	49,49,49,49	0
4	CL	G	2578	1/1	0.95	0.09	49,49,49,49	0
4	CL	K	2578	1/1	0.95	0.12	30,30,30,30	1
4	CL	C	2579	1/1	0.96	0.10	40,40,40,40	0
4	CL	M	2579	1/1	0.96	0.08	47,47,47,47	0
4	CL	M	2578	1/1	0.97	0.14	46,46,46,46	0
4	CL	G	2577	1/1	0.97	0.11	39,39,39,39	1
4	CL	A	2576	1/1	0.97	0.08	43,43,43,43	0
5	MG	K	2577	1/1	0.97	0.23	48,48,48,48	0
4	CL	K	2580	1/1	0.97	0.09	44,44,44,44	1
4	CL	M	2581	1/1	0.98	0.13	51,51,51,51	1
4	CL	C	2580	1/1	0.98	0.07	42,42,42,42	0
4	CL	K	2579	1/1	0.98	0.09	42,42,42,42	0
4	CL	E	2577	1/1	0.99	0.10	39,39,39,39	0
4	CL	A	2577	1/1	0.99	0.10	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.