



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 04:14 PM JST

PDB ID : 9JD0 / pdb\_00009jd0  
Title : Crystal structure of TMPRSS2 in complex with nanobody  
Authors : Wang, H.; Zhao, Z.; Liu, X.; Duan, Y.; Yang, H.  
Deposited on : 2024-08-30  
Resolution : 2.00 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

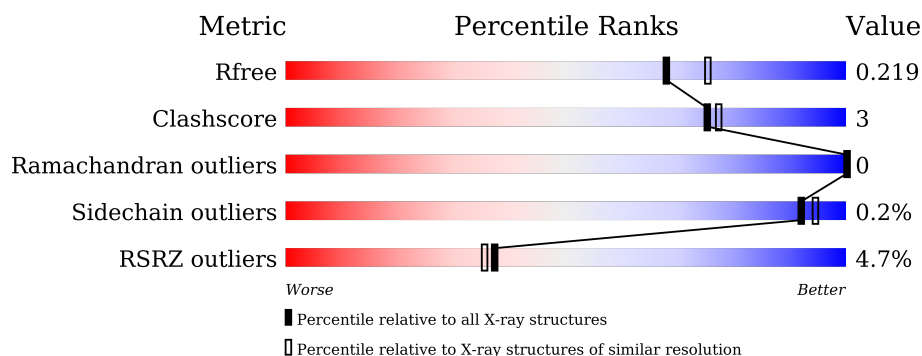
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	146	<div> <div>3%</div> <div>86% 8% 6%</div> </div>
1	B	146	<div> <div>11%</div> <div>88% 5% 6%</div> </div>
2	C	249	<div> <div>2%</div> <div>87% 9% .</div> </div>
2	D	249	<div> <div>%</div> <div>90% 5% .</div> </div>
3	E	131	<div> <div>5%</div> <div>89% 5% 7%</div> </div>
3	F	131	<div> <div>8%</div> <div>85% 7% 8%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8455 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 Transmembrane protease serine 2 non-catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	3	0
			1065	645	190	215	15			
1	B	137	Total	C	N	O	S	0	0	0
			1030	628	184	205	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ASP	SER	engineered mutation	UNP O15393
A	251	ASP	SER	engineered mutation	UNP O15393
A	252	ASP	ARG	engineered mutation	UNP O15393
A	253	ASP	GLN	engineered mutation	UNP O15393
A	254	LYS	SER	engineered mutation	UNP O15393
B	250	ASP	SER	engineered mutation	UNP O15393
B	251	ASP	SER	engineered mutation	UNP O15393
B	252	ASP	ARG	engineered mutation	UNP O15393
B	253	ASP	GLN	engineered mutation	UNP O15393
B	254	LYS	SER	engineered mutation	UNP O15393

- Molecule 2 is a protein called Transmembrane protease serine 2 catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	238	Total	C	N	O	S	0	6	0
			1880	1200	323	338	19			
2	D	238	Total	C	N	O	S	0	3	0
			1856	1187	318	334	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLU	-	expression tag	UNP O15393
C	494	PHE	-	expression tag	UNP O15393

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Chain	Residue	Modelled	Actual	Comment	Reference
C	495	VAL	-	expression tag	UNP O15393
C	496	GLU	-	expression tag	UNP O15393
C	497	HIS	-	expression tag	UNP O15393
C	498	HIS	-	expression tag	UNP O15393
C	499	HIS	-	expression tag	UNP O15393
C	500	HIS	-	expression tag	UNP O15393
C	501	HIS	-	expression tag	UNP O15393
C	502	HIS	-	expression tag	UNP O15393
C	503	HIS	-	expression tag	UNP O15393
C	504	HIS	-	expression tag	UNP O15393
D	493	GLU	-	expression tag	UNP O15393
D	494	PHE	-	expression tag	UNP O15393
D	495	VAL	-	expression tag	UNP O15393
D	496	GLU	-	expression tag	UNP O15393
D	497	HIS	-	expression tag	UNP O15393
D	498	HIS	-	expression tag	UNP O15393
D	499	HIS	-	expression tag	UNP O15393
D	500	HIS	-	expression tag	UNP O15393
D	501	HIS	-	expression tag	UNP O15393
D	502	HIS	-	expression tag	UNP O15393
D	503	HIS	-	expression tag	UNP O15393
D	504	HIS	-	expression tag	UNP O15393

- Molecule 3 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	120	Total	C	N	O	S	0	0	0
			915	572	161	177	5			
3	E	122	Total	C	N	O	S	0	1	0
			954	597	172	180	5			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

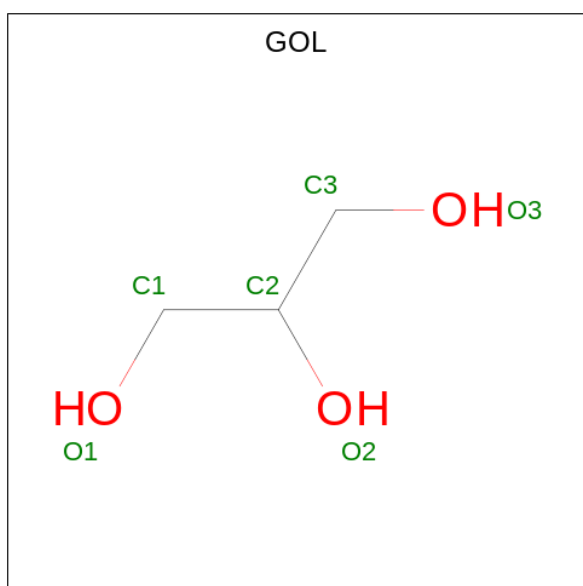
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



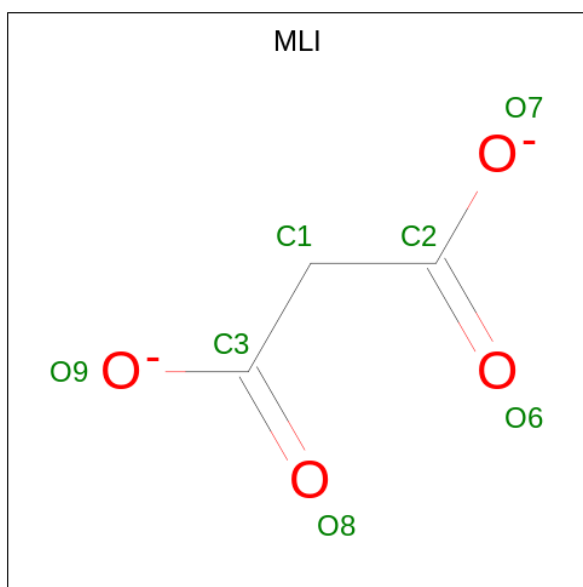
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	3	4		
7	D	1	Total	C	O	0	0
			7	3	4		
7	F	1	Total	C	O	0	0
			7	3	4		
7	E	1	Total	C	O	0	0
			7	3	4		

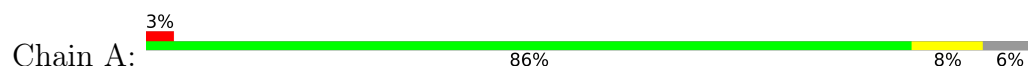
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	101	Total	O	0	0
			101	101		
8	B	73	Total	O	0	0
			73	73		
8	C	216	Total	O	0	0
			216	216		
8	D	192	Total	O	0	0
			192	192		
8	F	48	Total	O	0	0
			48	48		
8	E	61	Total	O	0	0
			61	61		

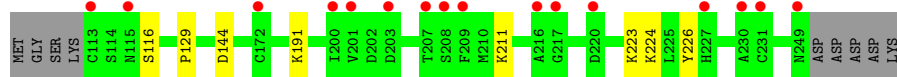
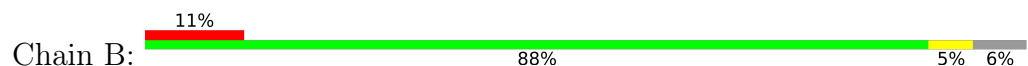
### 3 Residue-property plots [i](#)

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.

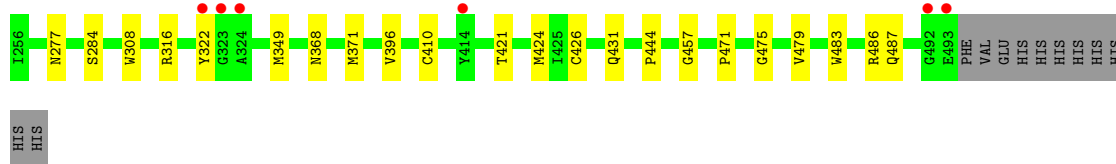
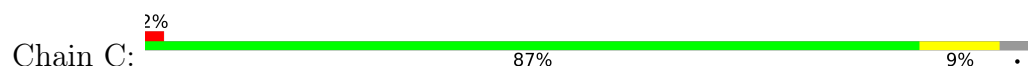
- Molecule 1: Transmembrane protease serine 2 non-catalytic chain



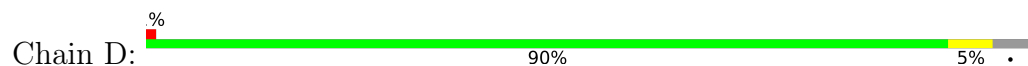
- Molecule 1: Transmembrane protease serine 2 non-catalytic chain



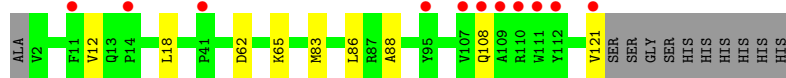
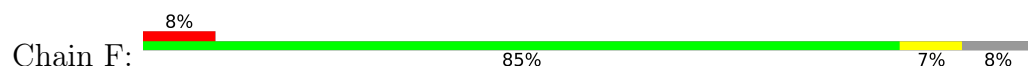
- Molecule 2: Transmembrane protease serine 2 catalytic chain



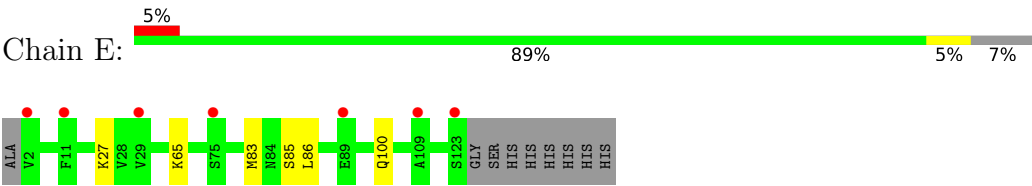
- Molecule 2: Transmembrane protease serine 2 catalytic chain



- Molecule 3: Nanobody



● Molecule 3: Nanobody





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.55Å 137.55Å 130.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.50 – 2.00 43.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.50-2.00) 99.9 (43.50-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (1.21_5207-000)	Depositor
R, $R_{free}$	0.188 , 0.221 0.188 , 0.219	Depositor DCC
$R_{free}$ test set	4267 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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 62.45 % 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 1.1245e-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 [i](#)

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

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

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	0.17	0/1087	0.33	0/1470
1	B	0.11	0/1052	0.29	0/1426
2	C	0.23	0/1937	0.45	0/2643
2	D	0.19	0/1913	0.44	0/2612
3	E	0.26	0/974	0.46	0/1319
3	F	0.16	0/933	0.35	0/1265
All	All	0.20	0/7896	0.40	0/10735

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 [i](#)

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	1065	0	964	6	0
1	B	1030	0	923	6	0
2	C	1880	0	1812	16	0
2	D	1856	0	1788	7	0
3	E	954	0	911	5	0
3	F	915	0	863	5	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	6	0	8	3	0
7	C	7	0	2	0	0
7	D	7	0	2	0	0
7	E	7	0	2	0	0
7	F	7	0	2	0	0
8	A	101	0	0	0	0
8	B	73	0	0	1	0
8	C	216	0	0	0	0
8	D	192	0	0	0	0
8	E	61	0	0	1	0
8	F	48	0	0	0	0
All	All	8455	0	7303	44	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 3.

All (44) 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)
2:C:410[B]:CYS:SG	2:C:426[B]:CYS:HB3	2.30	0.71
3:E:83:MET:HE2	3:E:86:LEU:HD21	1.74	0.68
3:E:100[A]:GLN:NE2	8:E:801:HOH:O	2.27	0.67
2:D:330:LYS:NZ	2:D:491:ASP:OD1	2.34	0.60
3:F:83:MET:HE2	3:F:86:LEU:HD21	1.81	0.60
3:F:88:ALA:HA	3:F:121:VAL:HG13	1.83	0.59
1:B:224:LYS:NZ	8:B:702:HOH:O	2.36	0.59
6:A:603:GOL:H12	2:C:486:ARG:HH12	1.72	0.55
2:C:316[A]:ARG:HG2	2:C:396:VAL:HG12	1.92	0.52
2:C:421:THR:OG1	2:C:424:MET:HG3	2.11	0.50
2:D:368:ASN:O	2:D:371:MET:HG2	2.12	0.49
1:B:223:LYS:HA	1:B:223:LYS:HD2	1.58	0.48
1:A:162:SER:HB2	1:A:210:MET:SD	2.54	0.47
1:A:170:PRO:HG2	1:A:209:PHE:HD1	1.80	0.47
2:C:426[B]:CYS:SG	2:C:471:PRO:HG2	2.54	0.47
2:C:368:ASN:O	2:C:371:MET:HG2	2.14	0.47
2:C:277[A]:ASN:ND2	2:C:322:TYR:HD1	2.13	0.46
1:A:132:TRP:CH2	6:A:603:GOL:H32	2.51	0.46
2:C:316[B]:ARG:HG2	2:C:396:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:65:LYS:HB3	3:E:65:LYS:HE2	1.65	0.46
1:A:208:SER:OG	1:A:227:HIS:NE2	2.47	0.45
2:C:483:TRP:O	2:C:487:GLN:HG2	2.17	0.44
2:D:311:PHE:CG	2:D:320:MET:HG2	2.53	0.44
6:A:603:GOL:H12	2:C:486:ARG:HH22	1.83	0.44
3:F:12:VAL:HG11	3:F:18:LEU:HG	2.00	0.43
3:E:85:SER:O	3:E:85:SER:OG	2.35	0.43
1:A:180:TYR:CE2	1:A:212:LEU:HD21	2.54	0.43
2:D:353:LYS:HA	2:D:354:PRO:HD3	1.88	0.43
3:E:27:LYS:HD2	3:E:27:LYS:HA	1.87	0.42
2:C:457:GLY:HA2	2:C:475:GLY:O	2.19	0.42
2:C:410[B]:CYS:SG	2:C:426[B]:CYS:CB	3.04	0.42
2:D:467:LYS:HE2	2:D:467:LYS:HB2	1.73	0.42
2:C:284:SER:OG	2:C:444:PRO:HB3	2.20	0.42
1:A:200:ILE:HD13	1:A:238:SER:HB2	2.01	0.41
3:F:108:GLN:N	3:F:108:GLN:OE1	2.53	0.41
1:B:144:ASP:OD1	1:B:144:ASP:N	2.51	0.41
2:C:277[A]:ASN:ND2	2:C:322:TYR:CD1	2.89	0.41
1:B:191:LYS:NZ	2:D:289:GLU:OE2	2.34	0.41
2:C:308:TRP:CD2	2:C:349:MET:HE1	2.57	0.40
1:B:116:SER:O	1:B:129:PRO:HG3	2.22	0.40
1:B:211:LYS:HE3	1:B:226:TYR:OH	2.21	0.40
3:F:62:ASP:OD1	3:F:65:LYS:HE2	2.21	0.40
2:C:431:GLN:CD	2:C:431:GLN:H	2.29	0.40
2:D:331:VAL:HG22	2:D:349:MET:HG2	2.03	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	138/146 (94%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	135/146 (92%)	129 (96%)	6 (4%)	0	100	100
2	C	242/249 (97%)	235 (97%)	7 (3%)	0	100	100
2	D	239/249 (96%)	230 (96%)	9 (4%)	0	100	100
3	E	121/131 (92%)	120 (99%)	1 (1%)	0	100	100
3	F	118/131 (90%)	117 (99%)	1 (1%)	0	100	100
All	All	993/1052 (94%)	965 (97%)	28 (3%)	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	122/127 (96%)	122 (100%)	0	100	100
1	B	113/127 (89%)	113 (100%)	0	100	100
2	C	202/210 (96%)	201 (100%)	1 (0%)	86	90
2	D	198/210 (94%)	197 (100%)	1 (0%)	86	90
3	E	97/107 (91%)	97 (100%)	0	100	100
3	F	92/107 (86%)	92 (100%)	0	100	100
All	All	824/888 (93%)	822 (100%)	2 (0%)	92	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	479	VAL
2	D	395	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN

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Mol	Chain	Res	Type
1	A	155	ASN
1	A	173	GLN
1	B	155	ASN
1	B	173	GLN
2	C	276	GLN
2	C	327	GLN
2	C	344	ASN
2	C	451	ASN
2	D	327	GLN
3	F	82	GLN
3	F	84	ASN
3	F	104	GLN
3	F	115	GLN
3	E	5	GLN
3	E	39	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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
7	MLI	F	800	-	6,6,6	1.68	1 (16%)	7,7,7	1.35	1 (14%)
6	GOL	A	603	-	5,5,5	0.08	0	5,5,5	0.47	0
7	MLI	C	900	-	6,6,6	1.55	1 (16%)	7,7,7	1.19	0
5	NAG	B	602	1	14,14,15	0.25	0	17,19,21	0.41	0
7	MLI	E	700	-	6,6,6	1.76	1 (16%)	7,7,7	1.10	0
7	MLI	D	600	-	6,6,6	1.57	1 (16%)	7,7,7	1.12	0
5	NAG	A	602	1	14,14,15	0.22	0	17,19,21	0.43	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
7	MLI	F	800	-	-	4/4/4/4	-
6	GOL	A	603	-	-	2/4/4/4	-
7	MLI	C	900	-	-	0/4/4/4	-
5	NAG	B	602	1	-	0/6/23/26	0/1/1/1
7	MLI	E	700	-	-	4/4/4/4	-
7	MLI	D	600	-	-	1/4/4/4	-
5	NAG	A	602	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	700	MLI	C1-C3	2.86	1.55	1.51
7	F	800	MLI	C1-C3	2.80	1.55	1.51
7	D	600	MLI	C1-C3	2.41	1.54	1.51
7	C	900	MLI	C1-C3	2.33	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	800	MLI	O6-C2-C1	-2.18	115.72	122.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	603	GOL	C1-C2-C3-O3
7	F	800	MLI	C3-C1-C2-O6
7	F	800	MLI	C3-C1-C2-O7
7	F	800	MLI	C2-C1-C3-O8
7	F	800	MLI	C2-C1-C3-O9
7	E	700	MLI	C2-C1-C3-O8
7	E	700	MLI	C3-C1-C2-O6
7	E	700	MLI	C3-C1-C2-O7
7	E	700	MLI	C2-C1-C3-O9
7	D	600	MLI	C2-C1-C3-O8

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	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

### 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	137/146 (93%)	0.12	4 (2%) 54 52	13, 33, 64, 94	7 (5%)
1	B	137/146 (93%)	0.66	16 (11%) 10 9	27, 41, 84, 99	0
2	C	238/249 (95%)	-0.24	6 (2%) 58 57	12, 27, 44, 68	10 (4%)
2	D	238/249 (95%)	-0.17	3 (1%) 74 73	12, 29, 46, 66	5 (2%)
3	E	122/131 (93%)	0.58	7 (5%) 30 28	13, 39, 60, 80	5 (4%)
3	F	120/131 (91%)	0.59	11 (9%) 16 15	22, 43, 69, 80	2 (1%)
All	All	992/1052 (94%)	0.15	47 (4%) 37 35	12, 33, 64, 99	29 (2%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	322	TYR	4.8
3	F	11	PHE	4.1
3	F	107	VAL	4.0
2	C	414	TYR	3.9
3	F	112	TYR	3.8
1	B	115	ASN	3.7
3	F	111	TRP	3.6
3	E	123	SER	3.5
3	F	121	VAL	3.1
2	D	493	GLU	3.1
3	F	41	PRO	3.0
2	C	323	GLY	3.0
3	F	109	ALA	3.0
1	B	217	GLY	2.8
3	F	108	GLN	2.8
3	E	89	GLU	2.8
1	A	217	GLY	2.7
1	B	231	CYS	2.6
2	C	493	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	11	PHE	2.6
1	B	230	ALA	2.6
1	B	201	VAL	2.6
1	B	200	ILE	2.5
3	F	110	ARG	2.5
1	A	115	ASN	2.5
2	D	492	GLY	2.5
1	A	207	THR	2.4
1	B	207	THR	2.4
1	B	209	PHE	2.4
1	B	113	CYS	2.3
3	E	29	VAL	2.3
2	C	492	GLY	2.3
1	B	172	CYS	2.3
3	E	75	SER	2.3
2	D	414	TYR	2.2
1	B	208	SER	2.2
1	B	216	ALA	2.2
2	C	324	ALA	2.2
1	B	249	ASN	2.2
1	B	203	ASP	2.1
3	F	14	PRO	2.1
1	A	248	LEU	2.1
3	E	109	ALA	2.1
1	B	220	ASP	2.1
1	B	227	HIS	2.1
3	E	2	VAL	2.1
3	F	95	TYR	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 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, 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
7	MLI	D	600	7/7	0.66	0.16	47,58,65,66	0
5	NAG	B	602	14/15	0.67	0.13	60,73,77,81	0
7	MLI	F	800	7/7	0.68	0.19	52,58,63,70	0
5	NAG	A	602	14/15	0.78	0.12	51,62,73,77	0
6	GOL	A	603	6/6	0.82	0.29	20,20,20,20	0
7	MLI	C	900	7/7	0.84	0.12	43,44,58,62	0
7	MLI	E	700	7/7	0.84	0.12	32,41,50,57	0
4	CA	A	601	1/1	0.98	0.04	22,22,22,22	0
4	CA	B	601	1/1	0.99	0.02	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.