



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:20 AM GMT

PDB ID : 3OPZ
Title : Crystal structure of trans-sialidase in complex with the Fab fragment of a neutralizing monoclonal IgG antibody
Authors : Larrieux, N.; Muia, R.; Campetella, O.; Buschiazzi, A.
Deposited on : 2010-09-02
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

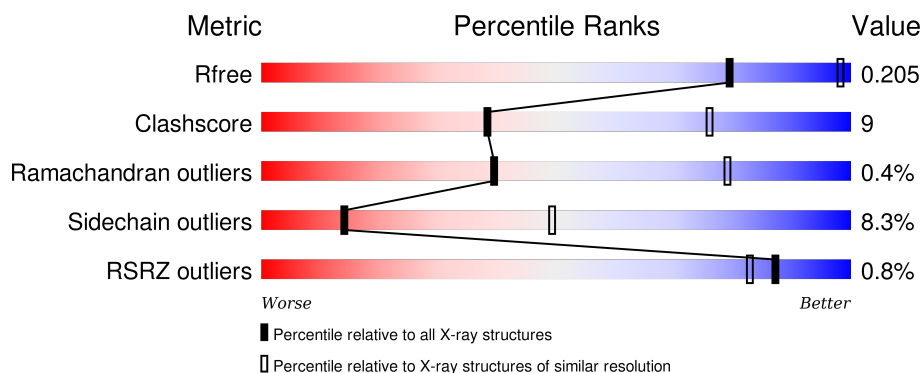
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	648	 78% 17% . .
1	B	648	 77% 18% . .
1	C	648	 78% 16% . .
2	H	222	 70% 23% 6% .
2	I	222	 69% 27% . .

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Mol	Chain	Length	Quality of chain
2	J	222	 4% 70% 25% •
3	L	213	 72% 23% 5% •
3	M	213	 72% 23% •
3	N	213	 % 76% 21% •

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
5	DIO	A	636	-	-	-	X
5	DIO	B	635	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24469 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 Trans-sialidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4858	3074	849	920	15			
1	B	625	Total	C	N	O	S	0	0	0
			4858	3074	849	920	15			
1	C	625	Total	C	N	O	S	0	0	0
			4858	3074	849	920	15			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q26966
A	-12	GLY	-	expression tag	UNP Q26966
A	-11	GLY	-	expression tag	UNP Q26966
A	-10	SER	-	expression tag	UNP Q26966
A	-9	HIS	-	expression tag	UNP Q26966
A	-8	HIS	-	expression tag	UNP Q26966
A	-7	HIS	-	expression tag	UNP Q26966
A	-6	HIS	-	expression tag	UNP Q26966
A	-5	HIS	-	expression tag	UNP Q26966
A	-4	HIS	-	expression tag	UNP Q26966
A	-3	GLY	-	expression tag	UNP Q26966
A	-2	MET	-	expression tag	UNP Q26966
A	-1	ALA	-	expression tag	UNP Q26966
A	0	SER	-	expression tag	UNP Q26966
A	58	PHE	ASN	engineered	UNP Q26966
A	262	THR	SER	see remark 999	UNP Q26966
A	476	HIS	ARG	see remark 999	UNP Q26966
A	484	LEU	VAL	see remark 999	UNP Q26966
A	495	LYS	SER	engineered	UNP Q26966
A	496	GLY	VAL	engineered	UNP Q26966
A	520	LYS	GLU	engineered	UNP Q26966
A	558	VAL	GLU	see remark 999	UNP Q26966
A	593	GLY	ASP	engineered	UNP Q26966

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Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASP	ILE	engineered	UNP Q26966
A	599	ARG	HIS	engineered	UNP Q26966
B	-13	MET	-	expression tag	UNP Q26966
B	-12	GLY	-	expression tag	UNP Q26966
B	-11	GLY	-	expression tag	UNP Q26966
B	-10	SER	-	expression tag	UNP Q26966
B	-9	HIS	-	expression tag	UNP Q26966
B	-8	HIS	-	expression tag	UNP Q26966
B	-7	HIS	-	expression tag	UNP Q26966
B	-6	HIS	-	expression tag	UNP Q26966
B	-5	HIS	-	expression tag	UNP Q26966
B	-4	HIS	-	expression tag	UNP Q26966
B	-3	GLY	-	expression tag	UNP Q26966
B	-2	MET	-	expression tag	UNP Q26966
B	-1	ALA	-	expression tag	UNP Q26966
B	0	SER	-	expression tag	UNP Q26966
B	58	PHE	ASN	engineered	UNP Q26966
B	262	THR	SER	engineered	UNP Q26966
B	476	HIS	ARG	engineered	UNP Q26966
B	484	LEU	VAL	engineered	UNP Q26966
B	495	LYS	SER	engineered	UNP Q26966
B	496	GLY	VAL	engineered	UNP Q26966
B	520	LYS	GLU	engineered	UNP Q26966
B	558	VAL	GLU	engineered	UNP Q26966
B	593	GLY	ASP	engineered	UNP Q26966
B	597	ASP	ILE	engineered	UNP Q26966
B	599	ARG	HIS	engineered	UNP Q26966
C	-13	MET	-	expression tag	UNP Q26966
C	-12	GLY	-	expression tag	UNP Q26966
C	-11	GLY	-	expression tag	UNP Q26966
C	-10	SER	-	expression tag	UNP Q26966
C	-9	HIS	-	expression tag	UNP Q26966
C	-8	HIS	-	expression tag	UNP Q26966
C	-7	HIS	-	expression tag	UNP Q26966
C	-6	HIS	-	expression tag	UNP Q26966
C	-5	HIS	-	expression tag	UNP Q26966
C	-4	HIS	-	expression tag	UNP Q26966
C	-3	GLY	-	expression tag	UNP Q26966
C	-2	MET	-	expression tag	UNP Q26966
C	-1	ALA	-	expression tag	UNP Q26966
C	0	SER	-	expression tag	UNP Q26966
C	58	PHE	ASN	engineered	UNP Q26966

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Chain	Residue	Modelled	Actual	Comment	Reference
C	262	THR	SER	engineered	UNP Q26966
C	476	HIS	ARG	engineered	UNP Q26966
C	484	LEU	VAL	engineered	UNP Q26966
C	495	LYS	SER	engineered	UNP Q26966
C	496	GLY	VAL	engineered	UNP Q26966
C	520	LYS	GLU	engineered	UNP Q26966
C	558	VAL	GLU	engineered	UNP Q26966
C	593	GLY	ASP	engineered	UNP Q26966
C	597	ASP	ILE	engineered	UNP Q26966
C	599	ARG	HIS	engineered	UNP Q26966

- Molecule 2 is a protein called heavy chain of the Fab fragment of immunoglobulin G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1639	1038	268	326	7			
2	I	220	Total	C	N	O	S	0	0	0
			1652	1051	268	326	7			
2	J	221	Total	C	N	O	S	0	0	0
			1653	1048	269	329	7			

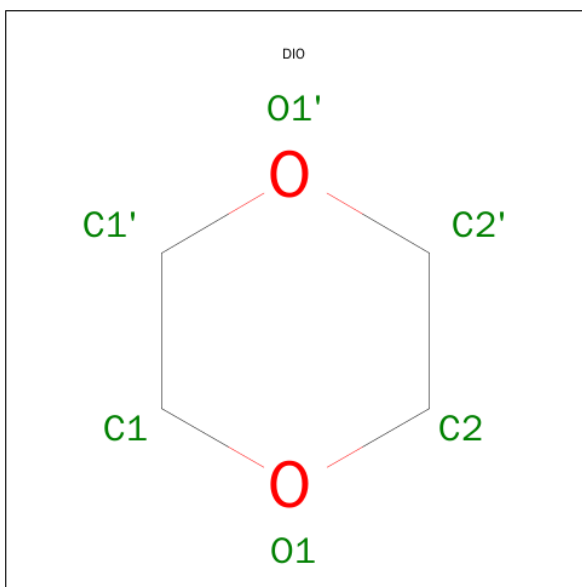
- Molecule 3 is a protein called light chain of the Fab fragment of immunoglobulin G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1632	1019	268	337	8			
3	M	212	Total	C	N	O	S	0	0	0
			1632	1019	268	337	8			
3	N	212	Total	C	N	O	S	0	0	0
			1632	1019	268	337	8			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		

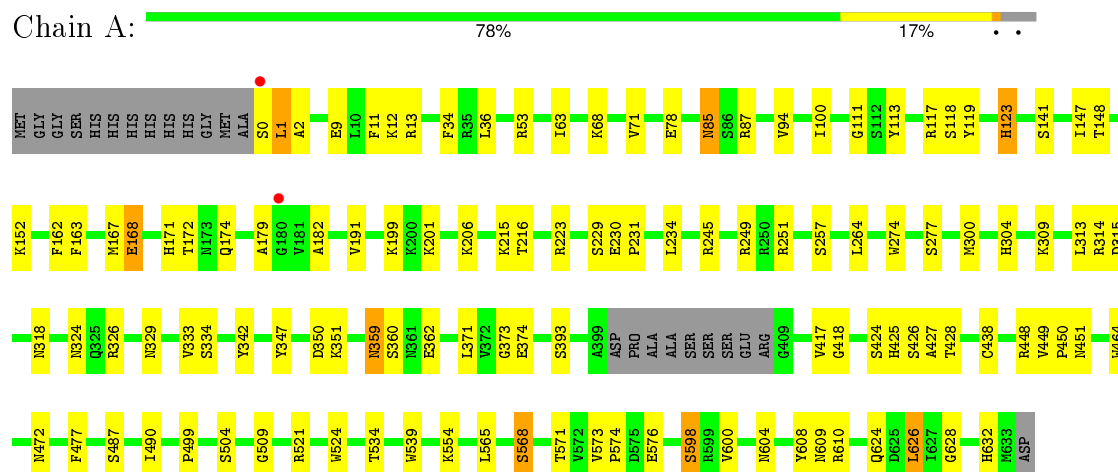
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	B	10	Total	O	0	0
			10	10		
6	C	5	Total	O	0	0
			5	5		
6	H	2	Total	O	0	0
			2	2		
6	J	1	Total	O	0	0
			1	1		
6	L	7	Total	O	0	0
			7	7		
6	M	3	Total	O	0	0
			3	3		
6	N	2	Total	O	0	0
			2	2		

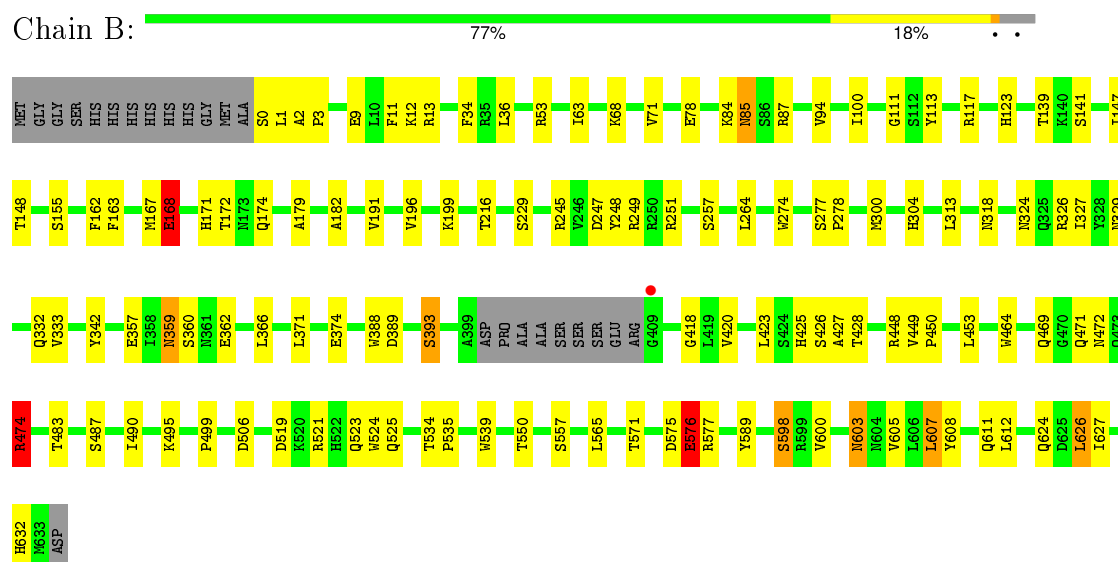
3 Residue-property plots

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

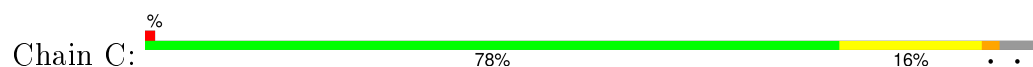
• Molecule 1: Trans-sialidase

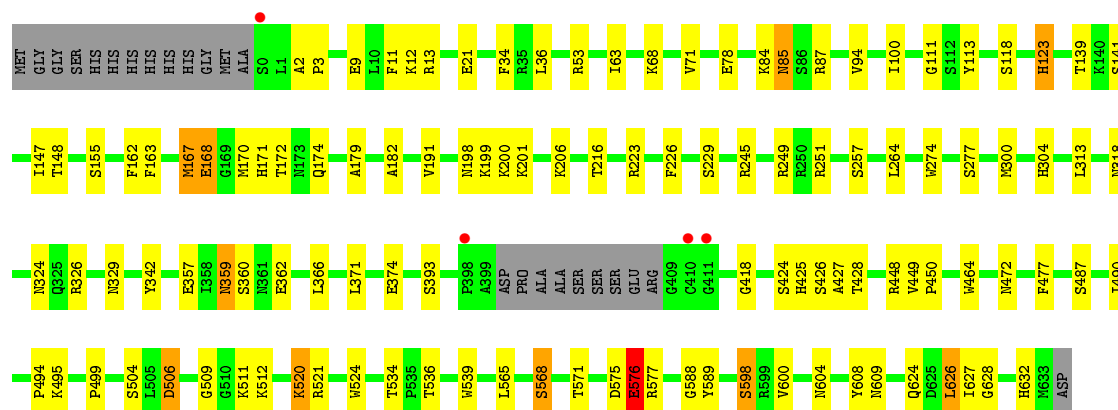


• Molecule 1: Trans-sialidase



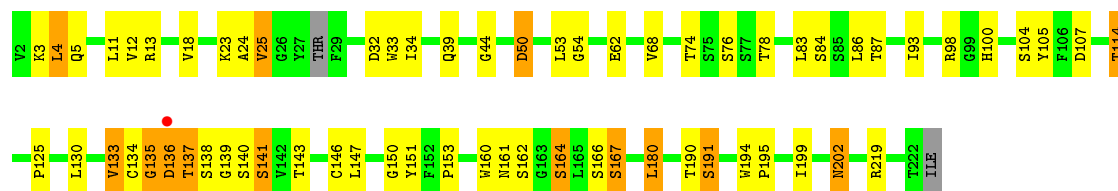
• Molecule 1: Trans-sialidase





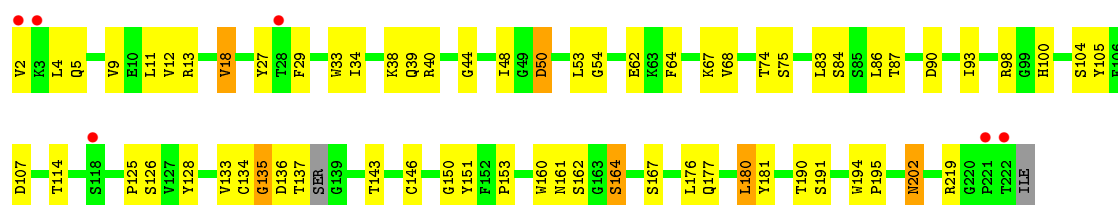
- Molecule 2: heavy chain of the Fab fragment of immunoglobulin G

Chain H: 70% 23% 6%



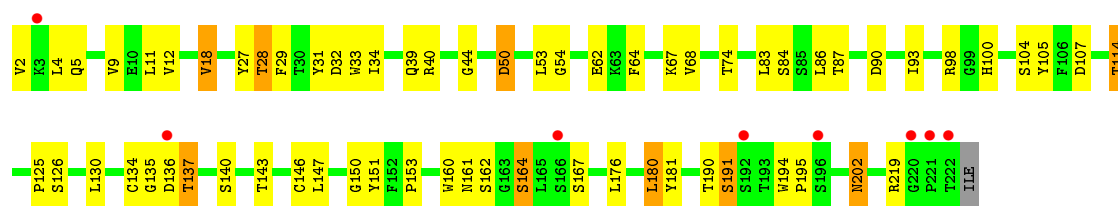
- Molecule 2: heavy chain of the Fab fragment of immunoglobulin G

Chain I: 69% 27% 3%



- Molecule 2: heavy chain of the Fab fragment of immunoglobulin G

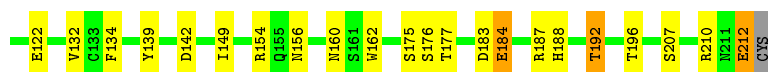
Chain J: 70% 25% 4%



- Molecule 3: light chain of the Fab fragment of immunoglobulin G

Chain L: 72% 23% 5%





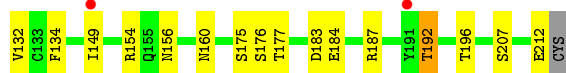
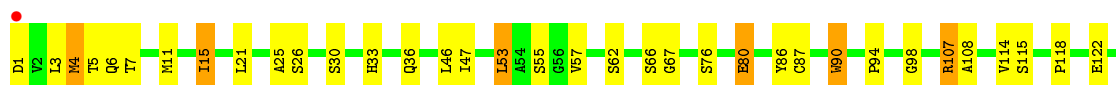
- Molecule 3: light chain of the Fab fragment of immunoglobulin G

Chain M: 72% 23% .



- Molecule 3: light chain of the Fab fragment of immunoglobulin G

Chain N: 76% 21% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	178.14Å 178.14Å 140.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.79 – 3.40 29.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.79-3.40) 100.0 (29.79-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, R_{free}	0.164 , 0.205 0.164 , 0.205	Depositor DCC
R_{free} test set	1014 reflections (1.50%)	DCC
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.2	EDS
Estimated twinning fraction	0.029 for -h,-k,l 0.048 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 68587 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24469	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, DIO

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	0.66	0/4971	0.77	4/6747 (0.1%)
1	B	0.64	1/4971 (0.0%)	0.77	2/6747 (0.0%)
1	C	0.61	1/4971 (0.0%)	0.74	2/6747 (0.0%)
2	H	0.65	0/1681	0.77	0/2296
2	I	0.60	0/1696	0.76	0/2317
2	J	0.59	0/1697	0.72	0/2320
3	L	0.66	0/1672	0.78	0/2273
3	M	0.65	0/1672	0.75	0/2273
3	N	0.58	0/1672	0.73	0/2273
All	All	0.63	2/25003 (0.0%)	0.76	8/33993 (0.0%)

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
2	I	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	576	GLU	CG-CD	6.13	1.61	1.51
1	B	0	SER	CA-CB	5.66	1.61	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	13	ARG	NE-CZ-NH2	-6.15	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	506	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	13	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	135	GLY	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	4858	0	4787	68	0
1	B	4858	0	4787	72	0
1	C	4858	0	4787	69	0
2	H	1639	0	1575	48	0
2	I	1652	0	1594	59	0
2	J	1653	0	1590	49	0
3	L	1632	0	1546	37	0
3	M	1632	0	1546	38	0
3	N	1632	0	1546	28	0
4	A	1	0	0	0	0
5	A	6	0	8	3	0
5	B	6	0	8	4	0
6	A	12	0	0	2	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	H	2	0	0	0	0
6	J	1	0	0	0	0
6	L	7	0	0	1	0
6	M	3	0	0	0	0
6	N	2	0	0	0	0
All	All	24469	0	23774	438	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 9.

The worst 5 of 438 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:J:2:VAL:CG2	2:J:27:TYR:CB	1.82	1.55
2:J:2:VAL:HG22	2:J:27:TYR:CB	1.10	1.53
2:J:140:SER:O	2:J:191:SER:HB2	1.10	1.27
2:J:140:SER:O	2:J:191:SER:CB	1.83	1.25
2:I:2:VAL:CG1	2:I:29:PHE:HE1	1.53	1.21

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	621/648 (96%)	586 (94%)	33 (5%)	2 (0%)	46	82
1	B	621/648 (96%)	589 (95%)	30 (5%)	2 (0%)	46	82
1	C	621/648 (96%)	590 (95%)	30 (5%)	1 (0%)	52	87
2	H	216/222 (97%)	199 (92%)	15 (7%)	2 (1%)	21	65
2	I	216/222 (97%)	201 (93%)	14 (6%)	1 (0%)	34	75
2	J	219/222 (99%)	201 (92%)	16 (7%)	2 (1%)	21	65
3	L	210/213 (99%)	197 (94%)	12 (6%)	1 (0%)	34	75
3	M	210/213 (99%)	201 (96%)	8 (4%)	1 (0%)	34	75
3	N	210/213 (99%)	199 (95%)	10 (5%)	1 (0%)	34	75
All	All	3144/3249 (97%)	2963 (94%)	168 (5%)	13 (0%)	39	79

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	135	GLY
2	I	135	GLY
2	J	135	GLY
3	L	67	GLY
3	M	67	GLY

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	529/547 (97%)	505 (96%)	24 (4%)	34	73
1	B	529/547 (97%)	495 (94%)	34 (6%)	22	62
1	C	529/547 (97%)	499 (94%)	30 (6%)	25	65
2	H	182/189 (96%)	161 (88%)	21 (12%)	7	31
2	I	184/189 (97%)	165 (90%)	19 (10%)	9	37
2	J	184/189 (97%)	163 (89%)	21 (11%)	7	31
3	L	188/190 (99%)	163 (87%)	25 (13%)	5	24
3	M	188/190 (99%)	161 (86%)	27 (14%)	4	21
3	N	188/190 (99%)	165 (88%)	23 (12%)	6	28
All	All	2701/2778 (97%)	2477 (92%)	224 (8%)	14	49

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	137	THR
2	I	190	THR
3	N	53	LEU
2	H	167	SER
2	I	13	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	318	ASN
1	C	604	ASN
3	M	189	ASN
1	C	324	ASN
1	C	359	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 carbohydrates 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$
5	DIO	A	636	-	6,6,6	1.29	0	6,6,6	0.72	0
5	DIO	B	635	-	6,6,6	1.64	2 (33%)	6,6,6	2.31	2 (33%)

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
5	DIO	A	636	-	-	0/0/6/6	0/1/1/1
5	DIO	B	635	-	-	0/0/6/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	635	DIO	O1'-C1'	2.53	1.53	1.42
5	B	635	DIO	O1-C2	2.60	1.53	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	635	DIO	C2'-O1'-C1'	3.23	120.75	109.89
5	B	635	DIO	C2-O1-C1	4.02	123.43	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	636	DIO	3	0
5	B	635	DIO	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	625/648 (96%)	-0.55	2 (0%) 94 92	25, 43, 66, 118	0
1	B	625/648 (96%)	-0.53	1 (0%) 95 94	27, 50, 75, 133	0
1	C	625/648 (96%)	-0.43	4 (0%) 90 86	34, 56, 84, 141	0
2	H	220/222 (99%)	-0.45	1 (0%) 91 89	35, 57, 102, 156	0
2	I	220/222 (99%)	-0.18	6 (2%) 58 53	50, 80, 123, 151	0
2	J	221/222 (99%)	0.22	8 (3%) 46 41	49, 95, 150, 184	0
3	L	212/213 (99%)	-0.62	0 100 100	31, 47, 70, 97	0
3	M	212/213 (99%)	-0.52	0 100 100	32, 50, 85, 122	0
3	N	212/213 (99%)	-0.10	3 (1%) 78 73	44, 72, 146, 169	0
All	All	3172/3249 (97%)	-0.41	25 (0%) 87 83	25, 54, 109, 184	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	222	THR	7.2
2	J	221	PRO	6.4
2	J	220	GLY	4.8
2	I	222	THR	4.1
2	J	166	SER	3.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	DIO	A	636	6/6	0.85	0.38	7.28	80,83,84,97	0
5	DIO	B	635	6/6	0.91	0.28	3.36	62,80,84,98	0
4	NA	A	635	1/1	0.87	0.39	-	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.