



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 03:08 PM EDT

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.; Buschiazzo, A.  
Deposited on : 2010-09-02  
Resolution : 3.40 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 : 2.23.2  
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) : 2.23.2

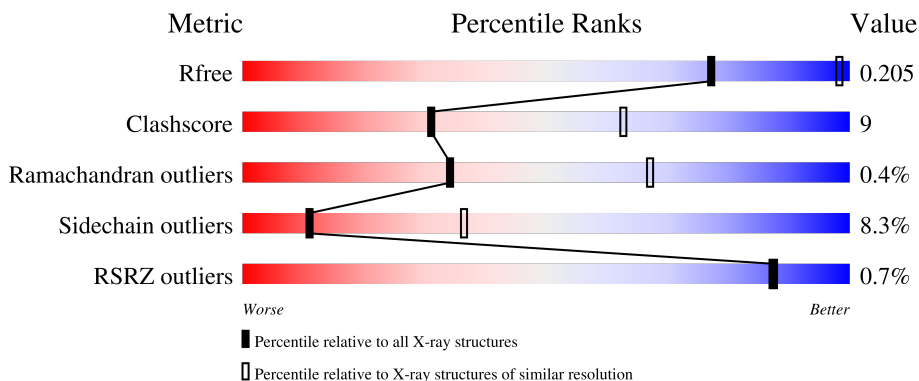
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (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 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	648	 78% 17% . .
1	B	648	 77% 18% . .
1	C	648	 78% 16% . .
2	H	222	 70% 23% 6% .
2	I	222	 3% 69% 27% . .

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

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	B	635	-	-	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
			Total	C	N	O	S			
1	A	625	4858	3074	849	920	15	0	0	0
1	B	625	4858	3074	849	920	15	0	0	0
1	C	625	4858	3074	849	920	15	0	0	0

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 mutation	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 mutation	UNP Q26966
A	496	GLY	VAL	engineered mutation	UNP Q26966
A	520	LYS	GLU	engineered mutation	UNP Q26966
A	558	VAL	GLU	see remark 999	UNP Q26966
A	593	GLY	ASP	engineered mutation	UNP Q26966

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

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

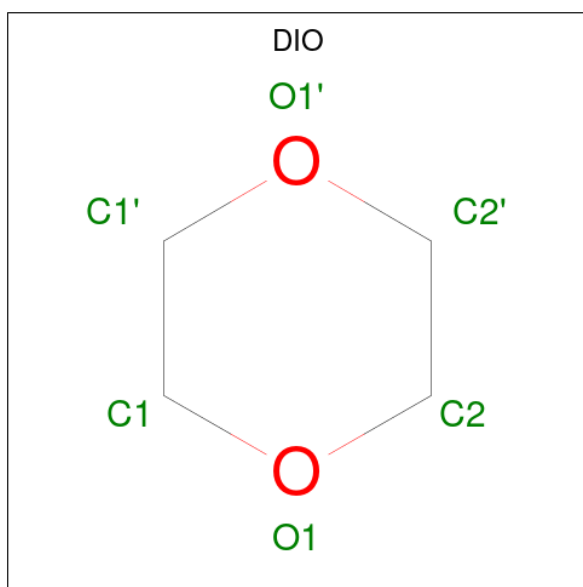
- Molecule 3 is a protein called light chain of the Fab fragment of immunoglobulin G.

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: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



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

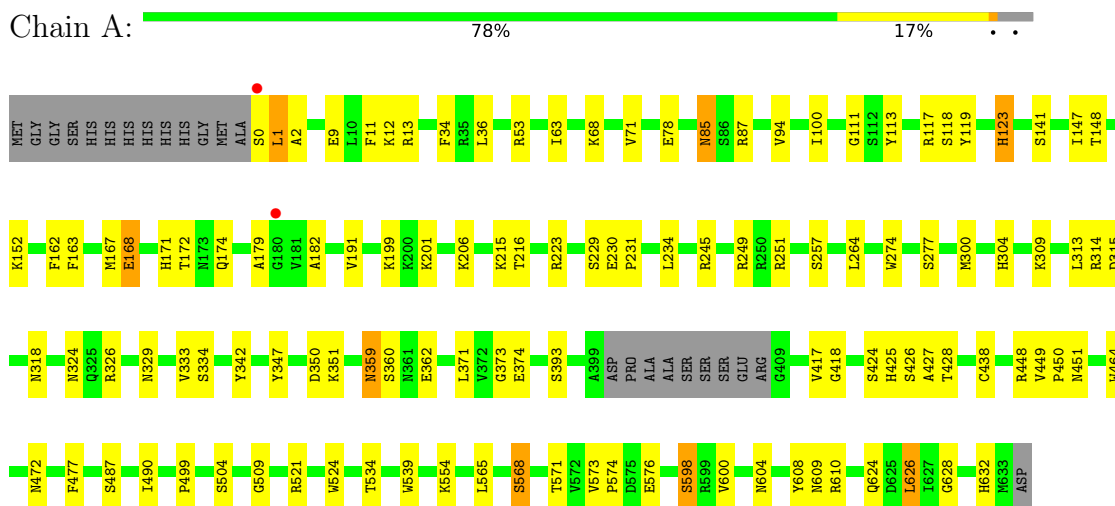
- Molecule 6 is water.

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

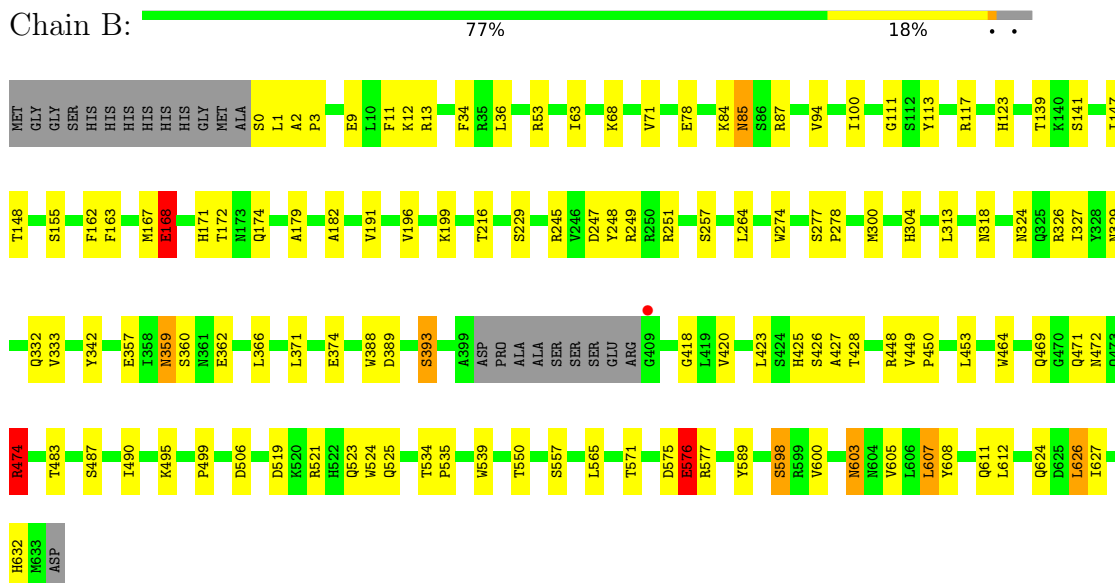
### 3 Residue-property plots [i](#)

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: Trans-sialidase




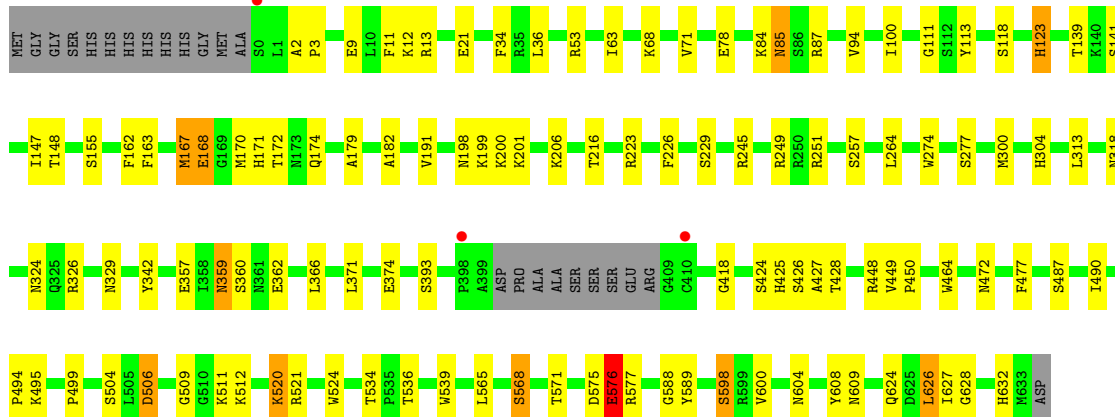
- Molecule 1: Trans-sialidase



- Molecule 1: Trans-sialidase

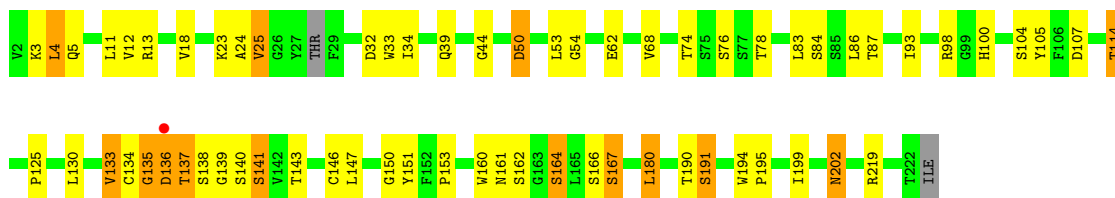


Chain C:  78% 16%



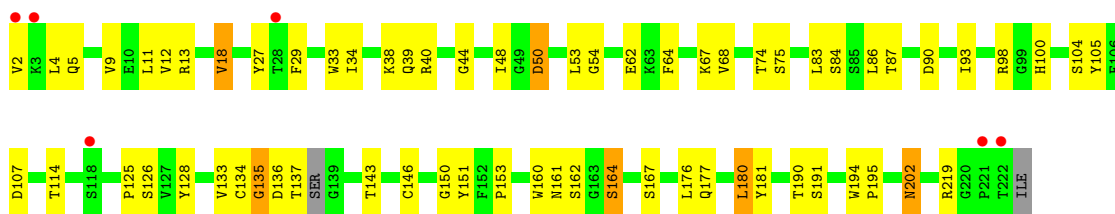
- Molecule 2: heavy chain of the Fab fragment of immunoglobulin G

Chain H:  70% 23% 6%



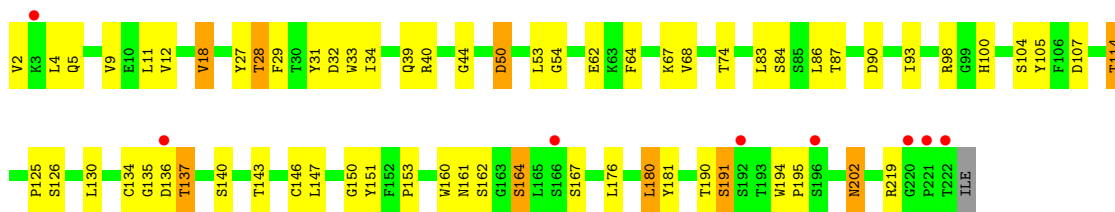
- Molecule 2: heavy chain of the Fab fragment of immunoglobulin G

Chain I:  3% 69% 27%



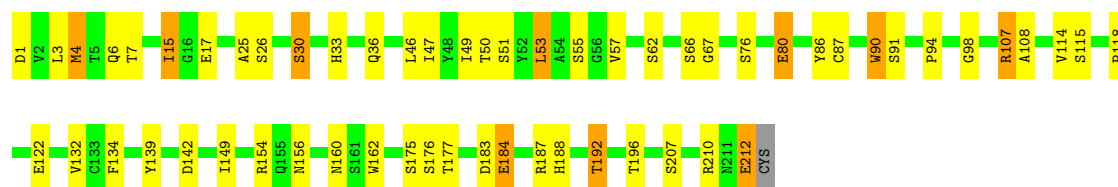
- Molecule 2: heavy chain of the Fab fragment of immunoglobulin G

Chain J:  4% 70% 25%



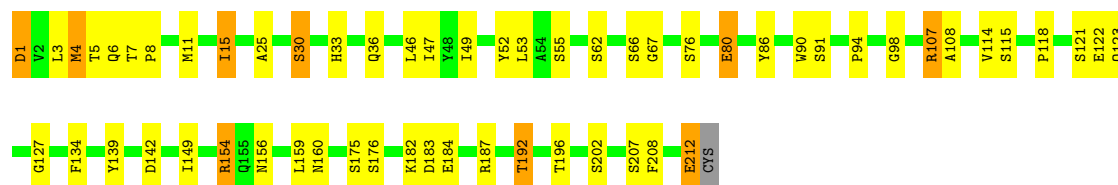
- Molecule 3: light chain of the Fab fragment of immunoglobulin G

Chain L:  72% 23% 5%




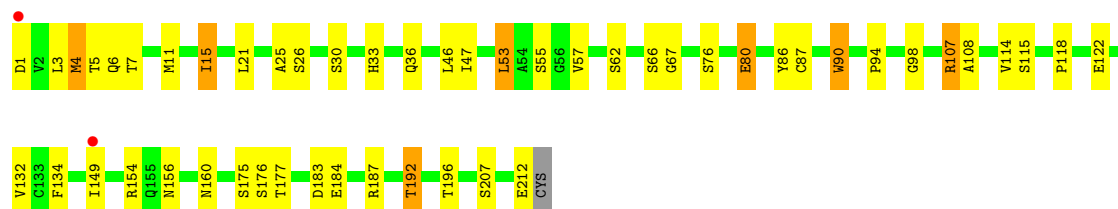
- Molecule 3: light chain of the Fab fragment of immunoglobulin G

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 3.39Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.164 , 0.205 0.164 , 0.205	Depositor DCC
$R_{free}$ test set	1014 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.029 for -h,-k,l 0.048 for h,-h-k,-l 0.035 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage'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.*

<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: DIO, NA

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

All (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
1	B	474	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	351	LYS	CD-CE-NZ	5.34	123.99	111.70
1	A	1	LEU	N-CA-C	-5.25	96.82	111.00

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 [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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:J:28:THR:CB	2:J:29:PHE:HA	1.77	1.12
2:I:2:VAL:CG1	2:I:29:PHE:CE1	2.34	1.09
2:I:2:VAL:HG11	2:I:29:PHE:CE1	1.92	1.03
2:H:23:LYS:NZ	2:H:76:SER:O	1.95	1.00
1:A:85:ASN:HD22	1:A:87:ARG:H	1.12	0.97
2:H:162:SER:H	2:H:202:ASN:HD21	1.14	0.96
1:B:575:ASP:OD1	1:B:577:ARG:HB2	1.67	0.95
2:J:2:VAL:CB	2:J:27:TYR:CB	2.45	0.94
2:I:162:SER:H	2:I:202:ASN:HD21	1.14	0.89
1:C:575:ASP:OD1	1:C:577:ARG:HB2	1.72	0.89
2:J:2:VAL:CA	2:J:27:TYR:CB	2.50	0.89
1:C:85:ASN:HD22	1:C:87:ARG:H	1.15	0.88
2:J:162:SER:H	2:J:202:ASN:HD21	1.15	0.88
2:H:4:LEU:HD13	2:H:24:ALA:HB2	1.54	0.87
2:I:48:ILE:HG23	2:I:64:PHE:HD2	1.39	0.87
2:I:2:VAL:HG13	2:I:29:PHE:HE1	1.40	0.86
1:B:85:ASN:HD22	1:B:87:ARG:H	1.18	0.85
2:I:219:ARG:NH1	3:M:118:PRO:HD2	1.93	0.83
2:H:136:ASP:OD1	2:H:138:SER:HA	1.78	0.83
2:J:140:SER:O	2:J:191:SER:CA	2.26	0.83
2:I:2:VAL:HG13	2:I:29:PHE:CE1	2.12	0.82
2:J:67:LYS:HE2	2:J:90:ASP:OD2	1.78	0.82
1:C:170:MET:CE	1:C:198:ASN:HD22	1.91	0.81
1:B:427:ALA:HB3	1:B:448:ARG:HD3	1.61	0.81
2:H:34:ILE:HD13	2:H:53:LEU:HD12	1.62	0.81
2:J:140:SER:C	2:J:191:SER:HB2	2.03	0.79
1:C:2:ALA:HB1	1:C:3:PRO:HD2	1.63	0.79
2:H:3:LYS:O	2:H:24:ALA:HB1	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:219:ARG:HH12	3:M:118:PRO:HD2	1.49	0.77
2:J:28:THR:CB	2:J:29:PHE:CA	2.57	0.77
2:H:3:LYS:O	2:H:24:ALA:CB	2.34	0.76
1:C:632:HIS:H	1:C:632:HIS:CD2	2.04	0.76
2:I:11:LEU:HD12	2:I:153:PRO:HG3	1.67	0.74
2:J:140:SER:O	2:J:191:SER:N	2.21	0.74
1:A:449:VAL:HB	1:A:450:PRO:HD2	1.69	0.74
1:B:1:LEU:HD13	1:B:333:VAL:O	1.88	0.74
1:A:632:HIS:CD2	1:A:632:HIS:H	2.04	0.74
3:N:6:GLN:HE22	3:N:86:TYR:HA	1.53	0.74
2:J:93:ILE:HG13	2:J:114:THR:HG23	1.70	0.73
2:H:93:ILE:HG13	2:H:114:THR:HG23	1.70	0.73
3:L:6:GLN:HE21	3:L:98:GLY:HA3	1.53	0.73
1:B:632:HIS:H	1:B:632:HIS:CD2	2.04	0.73
2:I:134:CYS:HB2	3:M:212:GLU:HB2	1.69	0.73
3:M:6:GLN:HE22	3:M:86:TYR:HA	1.53	0.72
1:C:170:MET:HE1	1:C:198:ASN:HD22	1.53	0.72
1:C:427:ALA:HB3	1:C:448:ARG:HD3	1.70	0.72
1:A:427:ALA:HB3	1:A:448:ARG:HD3	1.71	0.71
2:I:34:ILE:HD13	2:I:53:LEU:HD12	1.70	0.71
3:N:6:GLN:HE21	3:N:98:GLY:HA3	1.54	0.71
2:I:136:ASP:O	2:I:137:THR:HG22	1.90	0.71
3:M:6:GLN:HE21	3:M:98:GLY:HA3	1.55	0.71
3:L:6:GLN:HE22	3:L:86:TYR:HA	1.56	0.70
3:L:15:ILE:HD12	3:L:15:ILE:H	1.57	0.70
2:J:11:LEU:HD12	2:J:153:PRO:HG3	1.74	0.70
1:A:85:ASN:ND2	1:A:87:ARG:H	1.87	0.69
1:C:449:VAL:HB	1:C:450:PRO:HD2	1.74	0.68
1:B:449:VAL:HB	1:B:450:PRO:HD2	1.76	0.68
1:C:85:ASN:ND2	1:C:87:ARG:H	1.91	0.68
2:I:48:ILE:HG12	2:I:64:PHE:HE2	1.59	0.68
2:J:2:VAL:HA	2:J:27:TYR:CB	2.23	0.68
3:L:50:THR:HG22	3:L:51:SER:HB3	1.75	0.67
1:A:359:ASN:HD21	1:A:362:GLU:H	1.41	0.67
1:C:359:ASN:HD21	1:C:362:GLU:H	1.42	0.67
2:J:2:VAL:HG23	2:J:27:TYR:CB	2.12	0.67
3:N:4:MET:HB3	3:N:98:GLY:HA2	1.76	0.67
1:C:170:MET:HE2	1:C:198:ASN:HD22	1.60	0.66
3:M:15:ILE:HD12	3:M:15:ILE:H	1.60	0.66
3:L:4:MET:HB3	3:L:98:GLY:HA2	1.77	0.66
3:M:160:ASN:HD22	3:M:176:SER:HA	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:H	1:A:168:GLU:CD	1.99	0.65
1:B:342:TYR:OH	5:B:635:DIO:H1'1	1.95	0.65
3:M:1:ASP:N	3:M:94:PRO:HD2	2.12	0.65
1:B:359:ASN:HD21	1:B:362:GLU:H	1.44	0.65
3:N:15:ILE:H	3:N:15:ILE:HD12	1.61	0.65
1:A:2:ALA:HB1	1:A:373:GLY:HA3	1.79	0.65
2:H:166:SER:HB3	2:I:75:SER:HB3	1.79	0.64
2:I:93:ILE:HG13	2:I:114:THR:HG23	1.78	0.64
3:M:192:THR:HG23	3:M:207:SER:HB2	1.78	0.64
3:N:192:THR:HG23	3:N:207:SER:HB2	1.80	0.64
2:H:136:ASP:OD2	2:H:138:SER:HB2	1.98	0.63
3:M:4:MET:HB3	3:M:98:GLY:HA2	1.80	0.63
1:B:147:ILE:HD12	1:B:147:ILE:H	1.62	0.63
1:B:85:ASN:ND2	1:B:87:ARG:H	1.95	0.62
1:C:147:ILE:HD12	1:C:147:ILE:H	1.65	0.62
2:I:48:ILE:HG12	2:I:64:PHE:CE2	2.33	0.62
2:J:34:ILE:HD13	2:J:53:LEU:HD12	1.80	0.62
3:N:160:ASN:HD22	3:N:176:SER:HA	1.63	0.62
2:H:23:LYS:HB2	2:H:78:THR:HG23	1.82	0.62
3:L:192:THR:HG23	3:L:207:SER:HB2	1.81	0.62
2:I:134:CYS:CB	3:M:212:GLU:HB2	2.30	0.62
1:B:342:TYR:OH	5:B:635:DIO:C1'	2.48	0.62
1:C:565:LEU:O	1:C:568:SER:HB2	2.00	0.62
3:L:160:ASN:HD22	3:L:176:SER:HA	1.65	0.61
2:H:140:SER:O	2:H:141:SER:HB3	2.01	0.61
1:A:2:ALA:CB	1:A:373:GLY:HA3	2.30	0.61
2:I:2:VAL:HG22	2:I:27:TYR:CB	2.30	0.61
1:B:521:ARG:HB3	1:B:521:ARG:NH1	2.16	0.60
2:I:67:LYS:HE2	2:I:90:ASP:OD2	2.00	0.60
1:B:576:GLU:CD	1:B:576:GLU:H	2.04	0.60
2:J:2:VAL:N	2:J:27:TYR:CB	2.63	0.60
2:H:219:ARG:NH1	3:L:118:PRO:HD2	2.17	0.60
1:C:506:ASP:OD2	1:C:511:LYS:N	2.29	0.60
2:J:219:ARG:NH1	3:N:118:PRO:HD2	2.17	0.60
3:L:1:ASP:N	3:L:94:PRO:HD2	2.15	0.60
3:L:162:TRP:HB3	6:L:220:HOH:O	2.00	0.60
2:I:162:SER:N	2:I:202:ASN:HD21	1.94	0.60
2:H:98:ARG:NH2	2:H:107:ASP:OD2	2.35	0.60
1:C:576:GLU:OE2	1:C:576:GLU:HA	2.02	0.59
1:B:576:GLU:CD	1:B:576:GLU:N	2.56	0.59
2:J:162:SER:N	2:J:202:ASN:HD21	1.95	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:SER:OG	1:A:624:GLN:NE2	2.34	0.59
1:A:147:ILE:HD12	1:A:147:ILE:H	1.67	0.59
1:A:245:ARG:HH22	5:A:636:DIO:H22	1.68	0.59
2:J:98:ARG:NH2	2:J:107:ASP:OD2	2.36	0.59
1:A:314:ARG:HH22	5:A:636:DIO:H2'1	1.68	0.59
1:A:0:SER:O	1:A:334:SER:O	2.21	0.58
1:B:342:TYR:OH	5:B:635:DIO:O1'	2.21	0.58
1:C:575:ASP:OD1	1:C:577:ARG:CB	2.50	0.58
2:J:125:PRO:HB3	2:J:151:TYR:HB3	1.86	0.58
2:J:137:THR:HG23	2:J:137:THR:O	2.04	0.58
2:J:67:LYS:CE	2:J:90:ASP:OD2	2.52	0.57
2:H:137:THR:O	2:H:137:THR:CG2	2.53	0.57
2:I:133:VAL:HG21	3:M:208:PHE:HB2	1.87	0.57
3:N:1:ASP:N	3:N:94:PRO:HD2	2.19	0.57
3:L:3:LEU:O	3:L:3:LEU:HD12	2.05	0.57
2:I:125:PRO:HB3	2:I:151:TYR:HB3	1.87	0.57
1:B:519:ASP:HB3	1:B:525:GLN:HE21	1.69	0.57
1:C:487:SER:OG	1:C:624:GLN:NE2	2.38	0.57
1:A:1:LEU:HB3	6:A:642:HOH:O	2.05	0.56
2:I:105:TYR:HB3	3:M:33:HIS:CE1	2.40	0.56
2:H:139:GLY:O	2:H:140:SER:HB3	2.05	0.56
2:H:54:GLY:H	2:H:74:THR:HG21	1.70	0.56
2:J:33:TRP:CE3	2:J:50:ASP:HB2	2.41	0.56
1:B:521:ARG:HB3	1:B:521:ARG:HH11	1.70	0.56
2:H:137:THR:O	2:H:137:THR:HG23	2.05	0.56
1:B:487:SER:OG	1:B:624:GLN:NE2	2.38	0.56
1:B:469:GLN:OE1	1:B:474:ARG:HD2	2.06	0.56
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.87	0.56
1:A:1:LEU:HD13	1:A:333:VAL:O	2.06	0.56
2:I:136:ASP:O	2:I:137:THR:CG2	2.55	0.55
2:H:33:TRP:CE3	2:H:50:ASP:HB2	2.41	0.55
2:H:162:SER:N	2:H:202:ASN:HD21	1.94	0.55
1:B:575:ASP:OD1	1:B:577:ARG:N	2.32	0.55
3:M:1:ASP:H1	3:M:94:PRO:HD2	1.72	0.55
1:C:170:MET:CE	1:C:198:ASN:ND2	2.68	0.55
2:I:128:TYR:CZ	3:M:123:GLN:HG3	2.42	0.55
2:H:134:CYS:HB2	3:L:212:GLU:HB2	1.89	0.55
2:I:38:LYS:HE3	2:I:40:ARG:HD3	1.89	0.55
2:I:136:ASP:O	2:I:137:THR:CB	2.54	0.54
1:B:2:ALA:HB1	1:B:3:PRO:HD2	1.89	0.54
2:J:54:GLY:H	2:J:74:THR:HG21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:ASP:OD1	1:B:577:ARG:CB	2.49	0.54
1:B:359:ASN:HD22	1:B:360:SER:N	2.06	0.54
2:I:134:CYS:O	2:I:136:ASP:N	2.39	0.54
1:A:425:HIS:O	1:A:448:ARG:NH1	2.41	0.54
1:C:359:ASN:HD22	1:C:360:SER:N	2.06	0.54
2:I:98:ARG:NH2	2:I:107:ASP:OD2	2.41	0.54
3:N:3:LEU:HD12	3:N:3:LEU:O	2.08	0.53
1:B:425:HIS:O	1:B:448:ARG:NH1	2.41	0.53
1:C:576:GLU:OE2	1:C:576:GLU:CA	2.55	0.53
1:A:359:ASN:HD21	1:A:362:GLU:N	2.06	0.53
1:C:274:TRP:HA	1:C:472:ASN:HD22	1.74	0.53
2:I:105:TYR:HB3	3:M:33:HIS:NE2	2.23	0.53
2:I:48:ILE:HG23	2:I:64:PHE:CD2	2.31	0.53
1:A:167:MET:HG3	1:A:172:THR:CG2	2.39	0.53
1:C:425:HIS:O	1:C:448:ARG:NH1	2.42	0.53
1:A:274:TRP:HA	1:A:472:ASN:HD22	1.74	0.53
3:M:8:PRO:HD2	3:M:11:MET:HE2	1.91	0.53
1:C:576:GLU:OE2	1:C:576:GLU:N	2.42	0.53
3:N:1:ASP:H2	3:N:94:PRO:HD2	1.73	0.53
2:I:105:TYR:HB3	3:M:33:HIS:CD2	2.43	0.52
2:H:162:SER:H	2:H:202:ASN:ND2	1.96	0.52
3:N:107:ARG:HD3	3:N:108:ALA:O	2.09	0.52
1:A:565:LEU:O	1:A:568:SER:HB2	2.09	0.52
2:J:11:LEU:CD1	2:J:153:PRO:HG3	2.39	0.52
2:J:68:VAL:HG22	2:J:83:LEU:CD2	2.38	0.52
3:M:107:ARG:HD3	3:M:108:ALA:O	2.08	0.52
2:H:134:CYS:SG	3:L:212:GLU:HB2	2.49	0.52
3:L:3:LEU:HG	3:L:26:SER:HB3	1.92	0.52
2:H:68:VAL:HG22	2:H:83:LEU:CD2	2.40	0.52
2:J:134:CYS:O	2:J:136:ASP:N	2.43	0.52
2:H:134:CYS:O	2:H:135:GLY:O	2.28	0.51
2:H:32:ASP:OD2	2:H:98:ARG:HD2	2.10	0.51
2:I:177:GLN:OE1	3:M:159:LEU:HD11	2.10	0.51
1:C:575:ASP:OD1	1:C:577:ARG:N	2.36	0.51
2:H:134:CYS:CB	3:L:212:GLU:HB2	2.40	0.51
3:M:3:LEU:HD12	3:M:3:LEU:O	2.11	0.51
2:H:167:SER:HB2	2:I:75:SER:CB	2.41	0.51
3:L:1:ASP:H1	3:L:94:PRO:HD2	1.76	0.51
1:A:359:ASN:HD22	1:A:360:SER:N	2.09	0.51
2:H:98:ARG:HH21	2:H:107:ASP:CG	2.14	0.51
1:B:167:MET:CE	1:B:196:VAL:HG11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:161:ASN:O	2:J:164:SER:HB3	2.11	0.51
3:N:36:GLN:HB2	3:N:46:LEU:HD11	1.93	0.51
1:B:342:TYR:HH	5:B:635:DIO:C1'	2.22	0.51
3:L:49:ILE:O	3:L:49:ILE:HG22	2.10	0.51
3:M:36:GLN:HB2	3:M:46:LEU:HD11	1.93	0.51
1:B:274:TRP:HA	1:B:472:ASN:HD22	1.75	0.50
1:C:359:ASN:HD21	1:C:362:GLU:N	2.07	0.50
1:B:300:MET:CE	1:B:324:ASN:HB2	2.42	0.50
2:J:98:ARG:HH21	2:J:107:ASP:CG	2.15	0.50
2:I:161:ASN:O	2:I:164:SER:HB3	2.12	0.50
2:H:161:ASN:O	2:H:164:SER:HB3	2.11	0.50
3:L:107:ARG:HD3	3:L:108:ALA:O	2.12	0.50
2:I:54:GLY:H	2:I:74:THR:HG21	1.77	0.49
1:C:521:ARG:HB3	1:C:521:ARG:NH1	2.27	0.49
2:I:29:PHE:O	2:I:29:PHE:CD2	2.65	0.49
2:J:100:HIS:O	2:J:104:SER:HA	2.11	0.49
2:J:162:SER:H	2:J:202:ASN:ND2	1.97	0.49
1:B:359:ASN:HD21	1:B:362:GLU:N	2.09	0.49
1:B:327:ILE:HB	1:B:474:ARG:HG2	1.95	0.49
1:A:36:LEU:HD12	1:A:179:ALA:HB1	1.93	0.49
1:C:167:MET:O	1:C:168:GLU:C	2.51	0.49
1:A:504:SER:OG	1:A:509:GLY:HA2	2.11	0.49
1:C:170:MET:HE2	1:C:198:ASN:ND2	2.27	0.49
2:I:136:ASP:O	2:I:137:THR:HB	2.13	0.49
2:I:33:TRP:CE3	2:I:50:ASP:HB2	2.48	0.48
2:J:194:TRP:CG	2:J:195:PRO:HA	2.48	0.48
1:B:167:MET:O	1:B:168:GLU:C	2.51	0.48
1:B:575:ASP:HB2	1:B:576:GLU:OE2	2.13	0.48
2:H:105:TYR:HB3	3:L:33:HIS:CE1	2.48	0.48
2:I:68:VAL:HG22	2:I:83:LEU:CD2	2.42	0.48
2:I:98:ARG:HH21	2:I:107:ASP:CG	2.17	0.48
1:A:626:LEU:HD23	1:A:626:LEU:N	2.29	0.48
2:H:11:LEU:HD12	2:H:153:PRO:HG3	1.96	0.48
1:C:300:MET:CE	1:C:324:ASN:HB2	2.44	0.48
2:I:128:TYR:CE1	3:M:123:GLN:HG3	2.49	0.48
1:B:359:ASN:C	1:B:359:ASN:ND2	2.68	0.48
1:C:170:MET:HE1	1:C:198:ASN:ND2	2.27	0.48
2:I:100:HIS:O	2:I:104:SER:HA	2.14	0.48
1:A:167:MET:O	1:A:168:GLU:C	2.53	0.48
2:H:11:LEU:CD1	2:H:153:PRO:HG3	2.44	0.47
2:H:194:TRP:CG	2:H:195:PRO:HA	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:CD1	1:A:342:TYR:N	2.82	0.47
1:B:9:GLU:OE2	1:B:12:LYS:HG3	2.14	0.47
2:H:166:SER:CB	2:I:75:SER:HB3	2.44	0.47
1:A:521:ARG:NH1	1:A:521:ARG:HB3	2.29	0.47
1:C:2:ALA:HB1	1:C:3:PRO:CD	2.36	0.47
2:H:130:LEU:HD11	2:H:147:LEU:HB2	1.95	0.47
2:I:150:GLY:HA2	2:I:180:LEU:HD13	1.96	0.47
1:B:420:VAL:HB	1:B:607:LEU:HD23	1.96	0.47
1:C:424:SER:OG	1:C:604:ASN:ND2	2.48	0.47
1:C:626:LEU:N	1:C:626:LEU:HD23	2.30	0.47
1:B:603:ASN:OD1	1:B:603:ASN:N	2.47	0.47
2:I:2:VAL:CG1	2:I:29:PHE:CD1	2.96	0.47
3:N:80:GLU:O	3:N:80:GLU:HG2	2.14	0.47
1:C:9:GLU:OE2	1:C:12:LYS:HG3	2.15	0.47
1:C:21:GLU:OE1	1:C:84:LYS:HD3	2.14	0.47
2:H:219:ARG:HH12	3:L:118:PRO:HD2	1.78	0.47
2:I:194:TRP:CG	2:I:195:PRO:HA	2.50	0.47
2:J:150:GLY:HA2	2:J:180:LEU:HD13	1.96	0.47
3:L:36:GLN:HB2	3:L:46:LEU:HD11	1.97	0.47
1:C:499:PRO:HD2	1:C:598:SER:OG	2.14	0.47
2:J:219:ARG:HH12	3:N:118:PRO:HD2	1.79	0.47
3:M:15:ILE:H	3:M:15:ILE:CD1	2.26	0.47
2:J:105:TYR:HB3	3:N:33:HIS:CE1	2.49	0.47
1:B:167:MET:HE3	1:B:196:VAL:HG11	1.97	0.47
1:A:371:LEU:HB3	1:A:374:GLU:HB2	1.97	0.46
1:C:524:TRP:CZ2	1:C:539:TRP:HB3	2.50	0.46
1:C:359:ASN:C	1:C:359:ASN:ND2	2.68	0.46
2:I:162:SER:H	2:I:202:ASN:ND2	1.96	0.46
1:B:499:PRO:HD2	1:B:598:SER:OG	2.16	0.46
3:N:156:ASN:OD1	3:N:156:ASN:N	2.47	0.46
2:H:194:TRP:CD1	2:H:199:ILE:HD12	2.51	0.46
2:J:18:VAL:HG22	2:J:86:LEU:HD11	1.97	0.46
1:C:504:SER:OG	1:C:509:GLY:HA2	2.15	0.46
1:C:509:GLY:O	1:C:512:LYS:NZ	2.42	0.46
1:A:113:TYR:OH	1:A:174:GLN:NE2	2.49	0.46
1:A:417:VAL:HG23	1:A:610:ARG:HH21	1.80	0.46
2:J:34:ILE:HD13	2:J:53:LEU:CD1	2.46	0.46
1:B:524:TRP:CZ2	1:B:539:TRP:HB3	2.50	0.46
1:C:342:TYR:N	1:C:342:TYR:CD1	2.84	0.46
1:C:371:LEU:HB3	1:C:374:GLU:HB2	1.98	0.46
2:H:44:GLY:HA2	3:L:86:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HA	1:B:111:GLY:O	2.17	0.45
1:A:11:PHE:HB3	1:A:34:PHE:CG	2.51	0.45
1:A:300:MET:CE	1:A:324:ASN:HB2	2.46	0.45
1:A:438:CYS:HB2	6:A:644:HOH:O	2.15	0.45
1:B:53:ARG:HG2	1:B:63:ILE:HG12	1.98	0.45
1:B:371:LEU:HB3	1:B:374:GLU:HB2	1.98	0.45
1:C:575:ASP:OD2	1:C:577:ARG:NH2	2.49	0.45
1:B:523:GLN:OE1	1:B:535:PRO:HB2	2.16	0.45
1:C:494:PRO:O	1:C:520:LYS:HB3	2.16	0.45
1:A:424:SER:OG	1:A:604:ASN:ND2	2.49	0.45
2:I:18:VAL:HG22	2:I:86:LEU:HD11	1.98	0.45
3:M:1:ASP:H2	3:M:94:PRO:HD2	1.81	0.45
3:N:3:LEU:HG	3:N:26:SER:HB3	1.99	0.45
1:A:206:LYS:HD3	1:A:223:ARG:HB3	1.98	0.45
1:B:626:LEU:N	1:B:626:LEU:HD23	2.32	0.45
1:C:36:LEU:HD12	1:C:179:ALA:HB1	1.98	0.45
2:H:100:HIS:O	2:H:104:SER:HA	2.16	0.45
2:H:146:CYS:HB2	2:H:160:TRP:CH2	2.52	0.45
3:L:33:HIS:CE1	3:L:49:ILE:H	2.35	0.45
1:A:554:LYS:HB3	1:A:573:VAL:HB	1.99	0.45
1:A:167:MET:SD	1:A:206:LYS:HE2	2.57	0.44
2:H:136:ASP:OD1	2:H:138:SER:CA	2.56	0.44
2:I:44:GLY:HA2	3:M:86:TYR:OH	2.17	0.44
1:A:499:PRO:HD2	1:A:598:SER:OG	2.18	0.44
1:B:117:ARG:HG2	3:M:52:TYR:OH	2.17	0.44
1:C:170:MET:HE1	1:C:226:PHE:CE2	2.52	0.44
1:B:171:HIS:HB2	1:B:199:LYS:HG2	2.00	0.44
1:C:113:TYR:OH	1:C:174:GLN:NE2	2.50	0.44
1:C:94:VAL:HA	1:C:111:GLY:O	2.18	0.44
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.98	0.44
2:J:27:TYR:O	2:J:28:THR:C	2.56	0.44
1:A:359:ASN:C	1:A:359:ASN:ND2	2.70	0.44
2:I:137:THR:HG23	2:I:137:THR:O	2.17	0.44
3:N:4:MET:HG2	3:N:87:CYS:SG	2.58	0.44
1:C:53:ARG:HG2	1:C:63:ILE:HG12	1.99	0.44
3:L:53:LEU:HD21	3:L:57:VAL:O	2.18	0.44
3:M:127:GLY:O	3:M:182:LYS:HB2	2.18	0.44
1:A:425:HIS:HA	1:A:451:ASN:HA	1.99	0.44
1:A:490:ILE:HA	1:A:600:VAL:HG12	2.00	0.44
1:C:11:PHE:HB3	1:C:34:PHE:CG	2.53	0.44
2:H:139:GLY:HA2	2:H:191:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:PRO:HG3	1:B:589:TYR:CE1	2.53	0.43
1:A:251:ARG:HD2	1:A:304:HIS:CD2	2.53	0.43
1:B:36:LEU:HD12	1:B:179:ALA:HB1	2.00	0.43
1:C:499:PRO:HG3	1:C:589:TYR:CE1	2.54	0.43
3:M:80:GLU:O	3:M:80:GLU:HG2	2.15	0.43
1:C:68:LYS:HA	1:C:78:GLU:O	2.19	0.43
1:C:318:ASN:ND2	1:C:329:ASN:OD1	2.51	0.43
2:I:2:VAL:HG11	2:I:29:PHE:CD1	2.48	0.43
1:B:490:ILE:HA	1:B:600:VAL:HG12	1.99	0.43
2:J:105:TYR:HB3	3:N:33:HIS:CD2	2.54	0.43
1:B:247:ASP:HB3	1:B:248:TYR:CD1	2.54	0.43
1:B:318:ASN:ND2	1:B:329:ASN:OD1	2.51	0.43
1:B:342:TYR:N	1:B:342:TYR:CD1	2.84	0.43
2:I:34:ILE:HD13	2:I:53:LEU:CD1	2.45	0.43
1:A:53:ARG:HG2	1:A:63:ILE:HG12	2.00	0.43
1:B:113:TYR:OH	1:B:174:GLN:NE2	2.52	0.43
1:B:162:PHE:CZ	1:B:216:THR:HA	2.54	0.43
2:I:64:PHE:HB3	2:I:68:VAL:HG23	2.01	0.43
2:I:176:LEU:HD13	2:I:181:TYR:CE2	2.53	0.43
3:L:30:SER:OG	3:L:91:SER:HB3	2.19	0.43
3:N:53:LEU:HD21	3:N:57:VAL:O	2.19	0.43
1:B:68:LYS:HA	1:B:78:GLU:O	2.18	0.43
1:A:182:ALA:HB1	1:A:191:VAL:O	2.19	0.43
1:B:100:ILE:CG1	1:B:182:ALA:HB3	2.49	0.43
1:C:201:LYS:NZ	3:N:90:TRP:O	2.52	0.42
1:C:490:ILE:HA	1:C:600:VAL:HG12	2.00	0.42
3:L:156:ASN:OD1	3:L:156:ASN:N	2.46	0.42
1:B:357:GLU:HA	1:B:366:LEU:HD23	2.01	0.42
1:C:206:LYS:HD3	1:C:223:ARG:HB3	2.01	0.42
1:C:251:ARG:HD2	1:C:304:HIS:CD2	2.55	0.42
1:A:119:TYR:OH	5:A:636:DIO:H12	2.19	0.42
1:B:550:THR:HB	1:B:611:GLN:HG3	2.01	0.42
2:H:133:VAL:HG22	2:H:135:GLY:H	1.84	0.42
3:M:4:MET:HE2	3:M:25:ALA:HA	2.00	0.42
1:B:11:PHE:HB3	1:B:34:PHE:CG	2.54	0.42
2:I:176:LEU:HD12	2:I:176:LEU:HA	1.87	0.42
1:A:604:ASN:HD21	1:A:628:GLY:HA2	1.85	0.42
2:J:176:LEU:HD13	2:J:181:TYR:CE2	2.54	0.42
3:L:107:ARG:HD2	3:L:139:TYR:CG	2.55	0.42
1:A:68:LYS:HA	1:A:78:GLU:O	2.19	0.42
2:J:146:CYS:HB2	2:J:160:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:CG1	1:A:182:ALA:HB3	2.50	0.42
1:A:418:GLY:O	1:A:608:TYR:HA	2.20	0.42
1:B:182:ALA:HB1	1:B:191:VAL:O	2.20	0.42
1:C:162:PHE:CZ	1:C:216:THR:HA	2.55	0.42
2:I:146:CYS:HB2	2:I:160:TRP:CH2	2.55	0.42
2:J:64:PHE:HB3	2:J:68:VAL:HG23	2.02	0.42
2:J:130:LEU:HD11	2:J:147:LEU:HB2	2.01	0.42
3:M:160:ASN:ND2	3:M:176:SER:OG	2.51	0.42
3:N:114:VAL:HA	3:N:134:PHE:O	2.20	0.42
1:B:389:ASP:O	1:B:393:SER:OG	2.38	0.42
3:L:4:MET:HG2	3:L:87:CYS:SG	2.60	0.42
3:N:4:MET:HE2	3:N:25:ALA:HA	2.00	0.42
1:A:201:LYS:NZ	3:L:90:TRP:O	2.53	0.41
1:C:100:ILE:CG1	1:C:182:ALA:HB3	2.49	0.41
1:C:229:SER:O	1:C:245:ARG:HB3	2.20	0.41
1:C:604:ASN:HD21	1:C:628:GLY:HA2	1.85	0.41
3:L:114:VAL:HA	3:L:134:PHE:O	2.20	0.41
1:A:524:TRP:CZ2	1:A:539:TRP:HB3	2.55	0.41
1:A:347:TYR:OH	1:A:350:ASP:OD2	2.32	0.41
1:B:423:LEU:HB2	1:B:605:VAL:HB	2.02	0.41
2:H:150:GLY:HA2	2:H:180:LEU:HD13	2.00	0.41
3:M:184:GLU:HA	3:M:187:ARG:NH1	2.35	0.41
3:N:132:VAL:HG22	3:N:177:THR:HG23	2.03	0.41
1:A:9:GLU:OE2	1:A:12:LYS:HG3	2.20	0.41
1:B:1:LEU:O	1:B:2:ALA:C	2.59	0.41
1:C:418:GLY:O	1:C:608:TYR:HA	2.20	0.41
2:J:44:GLY:HA2	3:N:86:TYR:OH	2.21	0.41
1:A:118:SER:O	1:A:123:HIS:HE1	2.04	0.41
1:A:171:HIS:HB2	1:A:199:LYS:HG2	2.02	0.41
1:B:163:PHE:CZ	1:B:172:THR:HB	2.55	0.41
1:B:418:GLY:O	1:B:608:TYR:HA	2.20	0.41
3:L:132:VAL:HG22	3:L:177:THR:HG23	2.03	0.41
3:M:156:ASN:OD1	3:M:156:ASN:N	2.46	0.41
3:N:184:GLU:HA	3:N:187:ARG:NH1	2.35	0.41
1:A:234:LEU:HD12	1:A:234:LEU:C	2.41	0.41
1:A:318:ASN:ND2	1:A:329:ASN:OD1	2.51	0.41
1:C:182:ALA:HB1	1:C:191:VAL:O	2.21	0.41
1:C:477:PHE:CE2	1:C:609:ASN:HA	2.55	0.41
2:J:176:LEU:HD12	2:J:176:LEU:HA	1.89	0.41
3:L:80:GLU:O	3:L:80:GLU:HG2	2.21	0.41
3:L:184:GLU:HA	3:L:187:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:33:HIS:CE1	3:M:49:ILE:H	2.39	0.41
1:A:168:GLU:CD	1:A:168:GLU:N	2.72	0.41
1:B:278:PRO:HA	1:B:471:GLN:HB2	2.03	0.41
1:A:163:PHE:CZ	1:A:172:THR:HB	2.56	0.41
1:A:477:PHE:CE2	1:A:609:ASN:HA	2.55	0.41
1:C:163:PHE:CZ	1:C:172:THR:HB	2.55	0.41
1:C:171:HIS:HB2	1:C:199:LYS:HG2	2.02	0.41
1:C:357:GLU:HA	1:C:366:LEU:HD23	2.03	0.41
2:J:31:TYR:O	2:J:32:ASP:CG	2.59	0.41
3:L:1:ASP:H2	3:L:94:PRO:HD2	1.85	0.41
3:L:4:MET:HE2	3:L:25:ALA:HA	2.02	0.41
3:M:107:ARG:HD2	3:M:139:TYR:CG	2.56	0.41
3:M:114:VAL:HA	3:M:134:PHE:O	2.21	0.41
3:M:154:ARG:HA	3:M:154:ARG:HD3	1.96	0.41
2:H:25:VAL:H	2:H:25:VAL:HG23	1.56	0.41
1:A:229:SER:O	1:A:245:ARG:HB3	2.21	0.40
1:A:230:GLU:N	1:A:231:PRO:CD	2.84	0.40
1:A:309:LYS:HE3	1:A:315:ASP:HB3	2.03	0.40
1:A:427:ALA:HB3	1:A:448:ARG:CD	2.45	0.40
1:A:162:PHE:CZ	1:A:216:THR:HA	2.56	0.40
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.53	0.40
1:B:229:SER:O	1:B:245:ARG:HB3	2.21	0.40
1:B:251:ARG:HD2	1:B:304:HIS:CD2	2.56	0.40
3:N:6:GLN:NE2	3:N:98:GLY:HA3	2.31	0.40
1:B:388:TRP:CE3	1:B:388:TRP:HA	2.57	0.40
2:I:137:THR:CG2	2:I:137:THR:O	2.70	0.40
3:L:6:GLN:NE2	3:L:87:CYS:H	2.19	0.40
3:N:11:MET:HE3	3:N:21:LEU:HA	2.02	0.40
1:B:359:ASN:HD22	1:B:359:ASN:C	2.25	0.40
1:C:118:SER:O	1:C:123:HIS:HE1	2.05	0.40
1:C:499:PRO:HG2	1:C:588:GLY:HA2	2.04	0.40
3:L:188:HIS:O	3:L:210:ARG:NH1	2.54	0.40
1:A:94:VAL:HA	1:A:111:GLY:O	2.21	0.40
1:B:448:ARG:HA	1:B:453:LEU:HD23	2.04	0.40
1:B:483:THR:HG21	1:B:612:LEU:HD12	2.02	0.40
3:M:30:SER:OG	3:M:91:SER:HB3	2.22	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	621/648 (96%)	586 (94%)	33 (5%)	2 (0%)	41	72
1	B	621/648 (96%)	589 (95%)	30 (5%)	2 (0%)	41	72
1	C	621/648 (96%)	590 (95%)	30 (5%)	1 (0%)	47	78
2	H	216/222 (97%)	199 (92%)	15 (7%)	2 (1%)	17	49
2	I	216/222 (97%)	201 (93%)	14 (6%)	1 (0%)	29	61
2	J	219/222 (99%)	201 (92%)	16 (7%)	2 (1%)	17	49
3	L	210/213 (99%)	197 (94%)	12 (6%)	1 (0%)	29	61
3	M	210/213 (99%)	201 (96%)	8 (4%)	1 (0%)	29	61
3	N	210/213 (99%)	199 (95%)	10 (5%)	1 (0%)	29	61
All	All	3144/3249 (97%)	2963 (94%)	168 (5%)	13 (0%)	34	67

All (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
1	B	576	GLU
2	H	141	SER
3	N	67	GLY
1	A	168	GLU
1	A	574	PRO
2	J	28	THR
1	B	168	GLU
1	C	168	GLU

### 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	529/547 (97%)	505 (96%)	24 (4%)	27	58
1	B	529/547 (97%)	495 (94%)	34 (6%)	17	47
1	C	529/547 (97%)	499 (94%)	30 (6%)	20	50
2	H	182/189 (96%)	161 (88%)	21 (12%)	5	20
2	I	184/189 (97%)	165 (90%)	19 (10%)	7	26
2	J	184/189 (97%)	163 (89%)	21 (11%)	5	21
3	L	188/190 (99%)	163 (87%)	25 (13%)	4	15
3	M	188/190 (99%)	161 (86%)	27 (14%)	3	13
3	N	188/190 (99%)	165 (88%)	23 (12%)	5	18
All	All	2701/2778 (97%)	2477 (92%)	224 (8%)	11	36

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	85	ASN
1	A	117	ARG
1	A	123	HIS
1	A	141	SER
1	A	148	THR
1	A	152	LYS
1	A	215	LYS
1	A	249	ARG
1	A	257	SER
1	A	264	LEU
1	A	277	SER
1	A	326	ARG
1	A	359	ASN
1	A	393	SER
1	A	426	SER
1	A	428	THR
1	A	464	TRP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	534	THR
1	A	568	SER
1	A	571	THR
1	A	576	GLU
1	A	598	SER
1	A	626	LEU
1	B	71	VAL
1	B	84	LYS
1	B	85	ASN
1	B	123	HIS
1	B	139	THR
1	B	141	SER
1	B	148	THR
1	B	155	SER
1	B	168	GLU
1	B	249	ARG
1	B	257	SER
1	B	264	LEU
1	B	277	SER
1	B	313	LEU
1	B	326	ARG
1	B	332	GLN
1	B	359	ASN
1	B	393	SER
1	B	426	SER
1	B	428	THR
1	B	464	TRP
1	B	474	ARG
1	B	495	LYS
1	B	506	ASP
1	B	534	THR
1	B	557	SER
1	B	565	LEU
1	B	571	THR
1	B	576	GLU
1	B	598	SER
1	B	603	ASN
1	B	607	LEU
1	B	626	LEU
1	B	627	ILE
1	C	71	VAL
1	C	85	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	123	HIS
1	C	139	THR
1	C	141	SER
1	C	148	THR
1	C	155	SER
1	C	167	MET
1	C	200	LYS
1	C	249	ARG
1	C	257	SER
1	C	264	LEU
1	C	277	SER
1	C	313	LEU
1	C	326	ARG
1	C	359	ASN
1	C	393	SER
1	C	426	SER
1	C	428	THR
1	C	464	TRP
1	C	495	LYS
1	C	520	LYS
1	C	534	THR
1	C	536	THR
1	C	568	SER
1	C	571	THR
1	C	576	GLU
1	C	598	SER
1	C	626	LEU
1	C	627	ILE
2	H	4	LEU
2	H	5	GLN
2	H	12	VAL
2	H	13	ARG
2	H	25	VAL
2	H	39	GLN
2	H	50	ASP
2	H	62	GLU
2	H	84	SER
2	H	87	THR
2	H	114	THR
2	H	133	VAL
2	H	136	ASP
2	H	137	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	143	THR
2	H	164	SER
2	H	167	SER
2	H	180	LEU
2	H	190	THR
2	H	191	SER
2	H	202	ASN
2	I	4	LEU
2	I	5	GLN
2	I	9	VAL
2	I	12	VAL
2	I	13	ARG
2	I	18	VAL
2	I	39	GLN
2	I	50	ASP
2	I	62	GLU
2	I	84	SER
2	I	87	THR
2	I	126	SER
2	I	143	THR
2	I	164	SER
2	I	167	SER
2	I	180	LEU
2	I	190	THR
2	I	191	SER
2	I	202	ASN
2	J	4	LEU
2	J	5	GLN
2	J	9	VAL
2	J	12	VAL
2	J	18	VAL
2	J	39	GLN
2	J	40	ARG
2	J	50	ASP
2	J	62	GLU
2	J	84	SER
2	J	87	THR
2	J	114	THR
2	J	126	SER
2	J	137	THR
2	J	143	THR
2	J	164	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	167	SER
2	J	180	LEU
2	J	190	THR
2	J	191	SER
2	J	202	ASN
3	L	4	MET
3	L	7	THR
3	L	15	ILE
3	L	17	GLU
3	L	30	SER
3	L	47	ILE
3	L	53	LEU
3	L	55	SER
3	L	62	SER
3	L	66	SER
3	L	76	SER
3	L	80	GLU
3	L	90	TRP
3	L	107	ARG
3	L	115	SER
3	L	122	GLU
3	L	142	ASP
3	L	149	ILE
3	L	154	ARG
3	L	175	SER
3	L	183	ASP
3	L	184	GLU
3	L	192	THR
3	L	196	THR
3	L	212	GLU
3	M	1	ASP
3	M	4	MET
3	M	5	THR
3	M	7	THR
3	M	15	ILE
3	M	30	SER
3	M	47	ILE
3	M	53	LEU
3	M	55	SER
3	M	62	SER
3	M	66	SER
3	M	76	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	M	80	GLU
3	M	90	TRP
3	M	107	ARG
3	M	115	SER
3	M	121	SER
3	M	122	GLU
3	M	142	ASP
3	M	149	ILE
3	M	154	ARG
3	M	175	SER
3	M	183	ASP
3	M	192	THR
3	M	196	THR
3	M	202	SER
3	M	212	GLU
3	N	4	MET
3	N	5	THR
3	N	7	THR
3	N	15	ILE
3	N	30	SER
3	N	47	ILE
3	N	53	LEU
3	N	55	SER
3	N	62	SER
3	N	66	SER
3	N	76	SER
3	N	80	GLU
3	N	90	TRP
3	N	107	ARG
3	N	115	SER
3	N	122	GLU
3	N	149	ILE
3	N	154	ARG
3	N	175	SER
3	N	183	ASP
3	N	192	THR
3	N	196	THR
3	N	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	123	HIS
1	A	174	GLN
1	A	318	ASN
1	A	324	ASN
1	A	329	ASN
1	A	359	ASN
1	A	472	ASN
1	A	546	HIS
1	A	604	ASN
1	A	624	GLN
1	A	632	HIS
1	B	85	ASN
1	B	123	HIS
1	B	174	GLN
1	B	318	ASN
1	B	329	ASN
1	B	359	ASN
1	B	472	ASN
1	B	624	GLN
1	B	632	HIS
1	C	85	ASN
1	C	123	HIS
1	C	174	GLN
1	C	198	ASN
1	C	318	ASN
1	C	324	ASN
1	C	329	ASN
1	C	359	ASN
1	C	472	ASN
1	C	546	HIS
1	C	604	ASN
1	C	611	GLN
1	C	624	GLN
1	C	632	HIS
2	H	82	GLN
2	H	202	ASN
2	I	5	GLN
2	I	82	GLN
2	I	202	ASN
2	J	5	GLN
2	J	82	GLN
2	J	202	ASN

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Mol	Chain	Res	Type
3	L	6	GLN
3	L	155	GLN
3	L	160	ASN
3	L	189	ASN
3	M	6	GLN
3	M	31	HIS
3	M	155	GLN
3	M	160	ASN
3	M	189	ASN
3	N	6	GLN
3	N	155	GLN
3	N	160	ASN
3	N	189	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 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	B	635	-	6,6,6	1.68	2 (33%)	6,6,6	2.34	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DIO	A	636	-	6,6,6	1.33	0	6,6,6	0.73	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
5	DIO	B	635	-	-	-	0/1/1/1
5	DIO	A	636	-	-	-	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-C2	2.67	1.53	1.42
5	B	635	DIO	O1'-C1'	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	4.06	123.43	109.89
5	B	635	DIO	C2'-O1'-C1'	3.25	120.75	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	B	635	DIO	4	0
5	A	636	DIO	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	625/648 (96%)	-0.56	2 (0%) 94 93	25, 43, 66, 118	0
1	B	625/648 (96%)	-0.54	1 (0%) 95 95	27, 50, 75, 133	0
1	C	625/648 (96%)	-0.44	3 (0%) 91 90	34, 56, 84, 141	0
2	H	220/222 (99%)	-0.46	1 (0%) 91 90	35, 57, 102, 156	0
2	I	220/222 (99%)	-0.19	6 (2%) 54 53	50, 80, 123, 151	0
2	J	221/222 (99%)	0.20	8 (3%) 42 42	49, 95, 150, 184	0
3	L	212/213 (99%)	-0.63	0 100 100	31, 47, 70, 97	0
3	M	212/213 (99%)	-0.53	0 100 100	32, 50, 85, 122	0
3	N	212/213 (99%)	-0.11	2 (0%) 84 83	44, 72, 146, 169	0
All	All	3172/3249 (97%)	-0.42	23 (0%) 87 87	25, 54, 109, 184	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	222	THR	6.9
2	J	221	PRO	6.1
2	J	220	GLY	4.7
2	I	222	THR	4.0
2	J	166	SER	3.1
1	A	0	SER	2.9
2	I	221	PRO	2.8
2	J	136	ASP	2.6
3	N	149	ILE	2.5
2	I	2	VAL	2.5
2	H	136	ASP	2.5
1	C	410	CYS	2.4
2	J	3	LYS	2.3
1	A	180	GLY	2.2
2	I	3	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	0	SER	2.2
2	I	118	SER	2.1
3	N	1	ASP	2.1
2	I	28	THR	2.1
1	C	398	PRO	2.1
1	B	409	GLY	2.1
2	J	192	SER	2.1
2	J	196	SER	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

## 6.5 Other polymers [i](#)

There are no such residues in this entry.