



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:03 PM GMT

PDB ID : 5BZZ  
Title : Crystal structure of human phosphatase PTEN in its reduced state  
Authors : Lee, C.-U.; Bier, D.; Hennig, S.; Grossmann, T.N.  
Deposited on : 2015-06-11  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

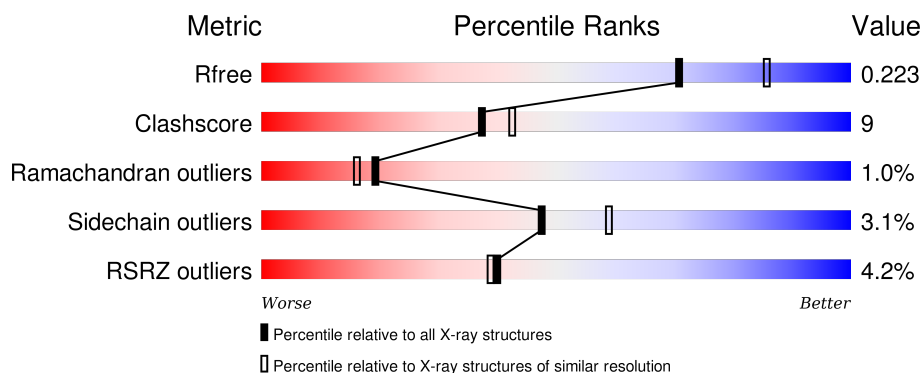
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	314	<div> <div>4%</div> <div>79%</div> <div>19%</div> </div>
1	B	314	<div> <div>8%</div> <div>75%</div> <div>20%</div> </div>
1	C	314	<div> <div>2%</div> <div>80%</div> <div>18%</div> </div>
1	D	314	<div> <div>3%</div> <div>77%</div> <div>21%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11268 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 Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2574	1669	436	453	16			
1	B	314	Total	C	N	O	S	0	0	0
			2562	1664	428	454	16			
1	C	314	Total	C	N	O	S	0	0	0
			2603	1684	440	463	16			
1	D	314	Total	C	N	O	S	0	0	0
			2599	1683	440	460	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	LYS	deletion	UNP P60484
A	?	-	VAL	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	ASN	deletion	UNP P60484
A	?	-	GLY	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484
A	?	-	LEU	deletion	UNP P60484
A	?	-	CYS	deletion	UNP P60484
A	?	-	ASP	deletion	UNP P60484
A	?	-	GLN	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	ILE	deletion	UNP P60484
A	?	-	ASP	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484
A	?	-	ILE	deletion	UNP P60484
A	?	-	CYS	deletion	UNP P60484
A	?	-	SER	deletion	UNP P60484

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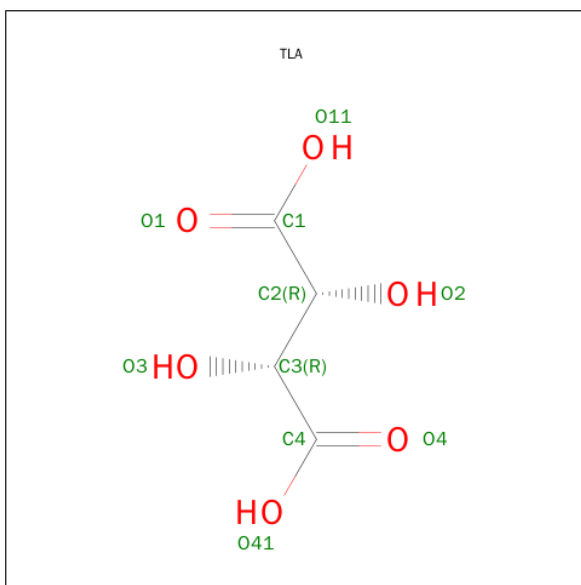
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P60484
A	?	-	GLU	deletion	UNP P60484
A	?	-	ARG	deletion	UNP P60484
A	?	-	ALA	deletion	UNP P60484
B	?	-	THR	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	LYS	deletion	UNP P60484
B	?	-	VAL	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	ASN	deletion	UNP P60484
B	?	-	GLY	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	LEU	deletion	UNP P60484
B	?	-	CYS	deletion	UNP P60484
B	?	-	ASP	deletion	UNP P60484
B	?	-	GLN	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	ILE	deletion	UNP P60484
B	?	-	ASP	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	ILE	deletion	UNP P60484
B	?	-	CYS	deletion	UNP P60484
B	?	-	SER	deletion	UNP P60484
B	?	-	ILE	deletion	UNP P60484
B	?	-	GLU	deletion	UNP P60484
B	?	-	ARG	deletion	UNP P60484
B	?	-	ALA	deletion	UNP P60484
C	?	-	THR	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484
C	?	-	LYS	deletion	UNP P60484
C	?	-	VAL	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484
C	?	-	ASN	deletion	UNP P60484
C	?	-	GLY	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	LEU	deletion	UNP P60484
C	?	-	CYS	deletion	UNP P60484
C	?	-	ASP	deletion	UNP P60484
C	?	-	GLN	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ILE	deletion	UNP P60484
C	?	-	ASP	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	ILE	deletion	UNP P60484
C	?	-	CYS	deletion	UNP P60484
C	?	-	SER	deletion	UNP P60484
C	?	-	ILE	deletion	UNP P60484
C	?	-	GLU	deletion	UNP P60484
C	?	-	ARG	deletion	UNP P60484
C	?	-	ALA	deletion	UNP P60484
D	?	-	THR	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	LYS	deletion	UNP P60484
D	?	-	VAL	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	ASN	deletion	UNP P60484
D	?	-	GLY	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	LEU	deletion	UNP P60484
D	?	-	CYS	deletion	UNP P60484
D	?	-	ASP	deletion	UNP P60484
D	?	-	GLN	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	ILE	deletion	UNP P60484
D	?	-	ASP	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	ILE	deletion	UNP P60484
D	?	-	CYS	deletion	UNP P60484
D	?	-	SER	deletion	UNP P60484
D	?	-	ILE	deletion	UNP P60484
D	?	-	GLU	deletion	UNP P60484
D	?	-	ARG	deletion	UNP P60484
D	?	-	ALA	deletion	UNP P60484

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	C	1	Total	C	O	0	0
			10	4	6		
2	D	1	Total	C	O	0	0
			10	4	6		

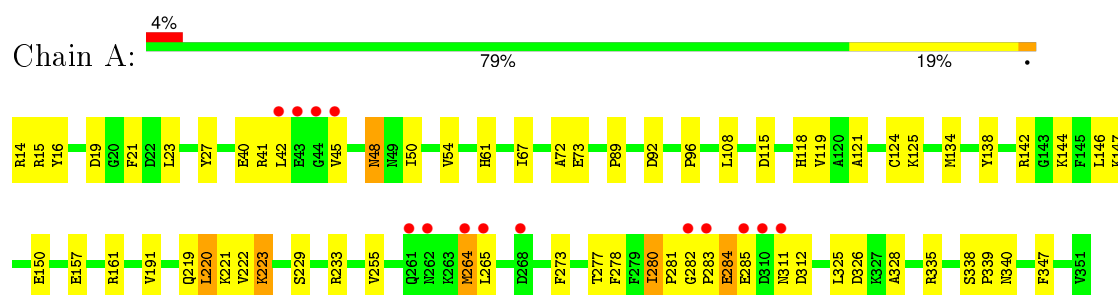
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total	O	0	0
			242	242		
3	B	242	Total	O	0	0
			242	242		
3	C	190	Total	O	0	0
			190	190		
3	D	216	Total	O	0	0
			216	216		

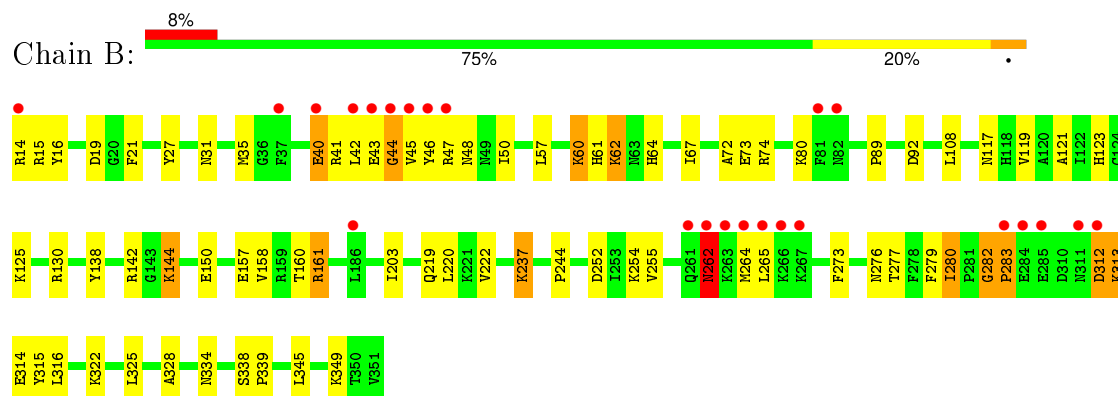
### 3 Residue-property plots

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.

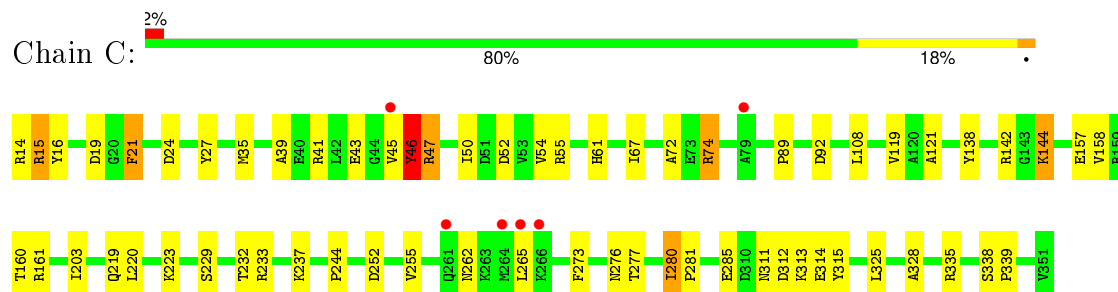
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



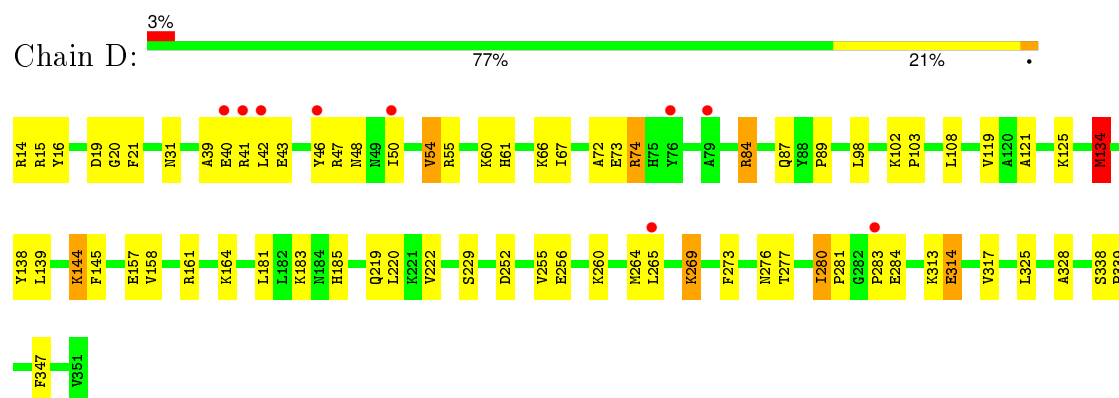
- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN



- Molecule 1: Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.17Å 207.39Å 87.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.36 – 2.20 46.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.36-2.20) 99.6 (46.36-2.20)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.192 , 0.221 0.193 , 0.223	Depositor DCC
$R_{free}$ test set	4795 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.3	EDS
Estimated twinning fraction	0.499 for H, K, L 0.501 for K, H, -L 0.488 for -k,-h,-l	Xtriage
Reported twinning fraction	0.499 for H, K, L 0.501 for K, H, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	4 of 95899 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.00 % 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 9.5681e-03. 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, 0.375 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: TLA

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	0.51	1/2649 (0.0%)	0.77	3/3581 (0.1%)
1	B	0.53	1/2637 (0.0%)	0.79	5/3570 (0.1%)
1	C	0.50	0/2679	0.81	7/3622 (0.2%)
1	D	0.50	0/2674	0.79	5/3612 (0.1%)
All	All	0.51	2/10639 (0.0%)	0.79	20/14385 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	7
1	C	0	2
1	D	0	8
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	GLY	C-O	6.87	1.34	1.23
1	A	280	ILE	C-O	-5.20	1.13	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	ARG	NE-CZ-NH2	11.58	126.09	120.30
1	C	15	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	D	134	MET	CG-SD-CE	7.01	111.41	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LEU	CA-CB-CG	6.55	130.36	115.30
1	C	280	ILE	N-CA-C	6.18	127.70	111.00
1	A	220	LEU	CB-CA-C	6.05	121.69	110.20
1	D	21	PHE	N-CA-C	-5.86	95.19	111.00
1	A	21	PHE	N-CA-C	-5.80	95.34	111.00
1	B	21	PHE	N-CA-C	-5.73	95.52	111.00
1	C	21	PHE	N-CA-C	-5.65	95.74	111.00
1	B	62	LYS	CA-CB-CG	5.62	125.77	113.40
1	C	46	TYR	CA-CB-CG	5.61	124.06	113.40
1	D	55	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	D	84	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	161	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	161	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	282	GLY	N-CA-C	-5.27	99.92	113.10
1	D	47	ARG	N-CA-C	5.22	125.11	111.00
1	C	47	ARG	N-CA-C	-5.05	97.35	111.00
1	C	46	TYR	CB-CA-C	5.02	120.43	110.40

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ASP	Peptide
1	A	264	MET	Peptide
1	A	265	LEU	Peptide
1	A	311	ASN	Peptide
1	A	312	ASP	Peptide
1	B	19	ASP	Peptide
1	B	262	ASN	Peptide
1	B	279	PHE	Peptide
1	B	280	ILE	Peptide
1	B	44	GLY	Peptide
1	B	46	TYR	Peptide
1	B	47	ARG	Peptide
1	C	19	ASP	Peptide
1	C	265	LEU	Peptide
1	D	19	ASP	Peptide
1	D	264	MET	Peptide
1	D	265	LEU	Peptide
1	D	280	ILE	Mainchain,Peptide
1	D	283	PRO	Mainchain,Peptide
1	D	46	TYR	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	2574	0	2485	60	0
1	B	2562	0	2454	60	0
1	C	2603	0	2514	43	2
1	D	2599	0	2527	41	2
2	A	10	0	4	2	0
2	B	10	0	4	1	0
2	C	10	0	4	1	0
2	D	10	0	4	0	0
3	A	242	0	0	3	0
3	B	242	0	0	6	0
3	C	190	0	0	4	1
3	D	216	0	0	7	1
All	All	11268	0	9996	189	3

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 (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:O	1:A:283:PRO:HD3	1.56	1.03
1:A:144:LYS:NZ	3:A:501:HOH:O	1.99	0.96
1:C:21:PHE:HA	3:C:510:HOH:O	1.66	0.96
1:A:283:PRO:O	1:A:285:GLU:N	2.01	0.94
1:A:280:ILE:O	1:A:283:PRO:CD	2.17	0.92
1:A:277:THR:O	1:A:281:PRO:HD3	1.76	0.86
1:A:280:ILE:O	1:A:283:PRO:CG	2.25	0.84
1:C:15:ARG:NH1	1:C:27:TYR:O	2.09	0.84
1:C:277:THR:HA	1:C:280:ILE:HD12	1.63	0.80
1:A:280:ILE:O	1:A:283:PRO:HG3	1.83	0.79
1:B:15:ARG:NH1	1:B:27:TYR:O	2.18	0.76
1:B:312:ASP:CB	1:B:315:TYR:HB2	2.18	0.73
1:B:73:GLU:HG3	1:B:74:ARG:HH21	1.54	0.71
1:D:256:GLU:OE2	1:D:269:LYS:HE3	1.90	0.71
1:C:15:ARG:HB2	1:C:158:VAL:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:OE2	1:B:125:LYS:HE3	1.92	0.69
1:B:64:HIS:CE1	1:B:117:ASN:HB2	2.28	0.69
1:A:220:LEU:HD12	1:A:221:LYS:H	1.57	0.69
1:A:326:ASP:O	3:A:502:HOH:O	2.11	0.69
1:C:24:ASP:OD2	1:C:47:ARG:NH2	2.26	0.68
1:A:150:GLU:OE1	1:B:161:ARG:NH1	2.27	0.68
1:A:281:PRO:C	1:A:283:PRO:HD3	2.15	0.67
1:A:277:THR:O	1:A:281:PRO:CD	2.41	0.67
1:A:282:GLY:N	1:A:283:PRO:CD	2.58	0.67
1:A:146:LEU:HD12	1:B:161:ARG:NH1	2.10	0.67
1:A:92:ASP:OD1	2:A:401:TLA:O2	2.05	0.66
1:A:146:LEU:H	1:B:161:ARG:HH22	1.41	0.66
1:D:15:ARG:HB2	1:D:158:VAL:O	1.97	0.65
1:B:73:GLU:HG3	1:B:74:ARG:NH2	2.11	0.65
1:A:45:VAL:CG2	1:A:125:LYS:HE3	2.26	0.65
1:C:338:SER:OG	1:C:339:PRO:O	2.14	0.65
1:B:62:LYS:NZ	3:B:512:HOH:O	2.31	0.64
1:D:20:GLY:O	3:D:502:HOH:O	2.14	0.64
1:B:73:GLU:OE2	1:B:125:LYS:CE	2.46	0.64
1:C:43:GLU:CD	1:C:74:ARG:HH22	2.00	0.64
1:A:161:ARG:NH1	1:B:150:GLU:OE2	2.31	0.63
1:D:134:MET:HA	1:D:134:MET:CE	2.28	0.62
1:B:161:ARG:HD2	3:B:617:HOH:O	1.99	0.62
1:C:39:ALA:HB1	1:C:43:GLU:HB3	1.82	0.62
1:D:338:SER:OG	1:D:339:PRO:O	2.14	0.62
1:C:43:GLU:OE1	1:C:74:ARG:NH2	2.33	0.62
1:D:220:LEU:N	3:D:506:HOH:O	2.31	0.61
1:B:254:LYS:NZ	3:B:515:HOH:O	2.32	0.61
1:B:50:ILE:HD13	1:B:80:LYS:HE3	1.83	0.61
1:A:338:SER:OG	1:A:339:PRO:O	2.15	0.60
1:B:40:GLU:OE1	1:B:43:GLU:HG3	2.02	0.60
1:B:277:THR:HA	1:B:280:ILE:HD12	1.84	0.59
1:B:338:SER:OG	1:B:339:PRO:O	2.14	0.59
1:B:244:PRO:HG3	1:D:222:VAL:HG21	1.85	0.59
1:D:256:GLU:OE2	1:D:269:LYS:CE	2.52	0.58
1:B:322:LYS:NZ	3:B:501:HOH:O	2.36	0.57
1:A:146:LEU:HD12	1:B:161:ARG:CZ	2.34	0.57
1:A:278:PHE:C	1:A:281:PRO:HD2	2.25	0.57
1:A:96:PRO:HG3	1:A:134:MET:HE1	1.87	0.57
1:A:278:PHE:O	1:A:281:PRO:HD2	2.03	0.57
1:A:282:GLY:N	1:A:283:PRO:HD3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:HG3	1:A:125:LYS:NZ	2.22	0.55
1:B:60:LYS:HG2	3:B:502:HOH:O	2.06	0.55
1:C:35:MET:HE3	1:C:121:ALA:HB1	1.88	0.55
1:B:92:ASP:OD1	2:B:401:TLA:O3	2.15	0.55
1:D:84:ARG:NH1	3:D:512:HOH:O	2.41	0.54
1:A:146:LEU:N	1:B:161:ARG:HH22	2.04	0.54
1:A:191:VAL:HG11	1:A:281:PRO:HG2	1.90	0.54
1:C:233:ARG:NH2	3:C:514:HOH:O	2.41	0.53
1:B:219:GLN:O	1:B:220:LEU:HB2	2.09	0.52
1:A:16:TYR:HE1	1:A:161:ARG:H	1.57	0.52
1:C:219:GLN:O	1:C:220:LEU:HB2	2.09	0.52
1:C:223:LYS:NZ	3:C:515:HOH:O	2.42	0.52
1:A:280:ILE:HD13	1:A:347:PHE:CE1	2.45	0.52
1:D:134:MET:HE2	1:D:134:MET:HA	1.92	0.52
1:B:15:ARG:HB2	1:B:158:VAL:O	2.10	0.52
1:D:314:GLU:O	1:D:314:GLU:HG2	2.10	0.52
1:D:219:GLN:O	1:D:220:LEU:HB2	2.10	0.51
1:C:67:ILE:HD13	1:C:121:ALA:HB3	1.93	0.51
1:C:92:ASP:OD1	2:C:401:TLA:O3	2.17	0.51
1:A:150:GLU:OE2	1:B:161:ARG:CZ	2.58	0.51
1:B:222:VAL:HG21	1:C:244:PRO:HG3	1.93	0.51
1:A:220:LEU:HD11	1:A:222:VAL:HG23	1.93	0.51
1:A:67:ILE:HD13	1:A:121:ALA:HB3	1.93	0.50
1:D:67:ILE:HD13	1:D:121:ALA:HB3	1.93	0.50
1:D:16:TYR:HE1	1:D:161:ARG:H	1.59	0.50
1:A:233:ARG:HA	3:A:572:HOH:O	2.11	0.50
1:A:40:GLU:O	1:A:42:LEU:N	2.45	0.50
1:C:16:TYR:HE1	1:C:161:ARG:H	1.60	0.50
1:B:67:ILE:HD13	1:B:121:ALA:HB3	1.94	0.50
1:A:15:ARG:HD3	1:B:144:LYS:NZ	2.27	0.50
1:C:52:ASP:OD1	1:C:55:ARG:NH2	2.45	0.49
1:A:281:PRO:CA	1:A:283:PRO:HD3	2.42	0.49
1:B:282:GLY:O	1:B:283:PRO:C	2.51	0.49
1:B:325:LEU:HB2	1:B:328:ALA:HB3	1.95	0.49
1:D:313:LYS:O	1:D:314:GLU:HB3	2.13	0.48
1:A:96:PRO:HG3	1:A:134:MET:CE	2.43	0.48
1:D:277:THR:HA	1:D:280:ILE:HD12	1.94	0.48
1:B:334:ASN:OD1	3:B:501:HOH:O	2.20	0.48
1:C:138:TYR:CZ	1:C:142:ARG:HG3	2.49	0.48
1:C:325:LEU:HB2	1:C:328:ALA:HB3	1.96	0.48
1:C:314:GLU:HB2	1:C:315:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:VAL:O	1:C:46:TYR:HB3	2.15	0.47
1:C:15:ARG:NH1	1:C:27:TYR:HB2	2.29	0.47
1:D:281:PRO:HB3	1:D:317:VAL:O	2.13	0.47
1:A:223:LYS:O	1:A:223:LYS:HG2	2.15	0.47
1:D:325:LEU:HB2	1:D:328:ALA:HB3	1.95	0.47
1:D:144:LYS:NZ	3:D:516:HOH:O	2.46	0.47
1:A:23:LEU:HA	1:A:48:ASN:HD21	1.79	0.47
1:C:16:TYR:CD1	1:C:161:ARG:HG3	2.50	0.47
1:B:72:ALA:HA	1:B:89:PRO:HB2	1.97	0.46
1:D:164:LYS:NZ	3:D:518:HOH:O	2.47	0.46
1:B:125:LYS:HE3	1:B:130:ARG:HH22	1.79	0.46
1:C:108:LEU:HD23	1:C:138:TYR:CG	2.50	0.46
1:D:72:ALA:HA	1:D:89:PRO:HB2	1.96	0.46
1:A:325:LEU:HB2	1:A:328:ALA:HB3	1.96	0.46
1:A:14:ARG:HA	1:A:161:ARG:HA	1.97	0.46
1:C:50:ILE:O	1:C:54:VAL:HG23	2.16	0.46
1:D:41:ARG:NH1	1:D:43:GLU:HA	2.30	0.46
1:B:16:TYR:HE1	1:B:161:ARG:H	1.62	0.46
1:C:144:LYS:HA	1:C:144:LYS:HD3	1.72	0.46
1:B:74:ARG:HH21	1:B:74:ARG:HG3	1.81	0.46
1:A:50:ILE:O	1:A:54:VAL:HG23	2.16	0.46
1:C:252:ASP:OD1	1:C:276:ASN:ND2	2.47	0.45
1:C:35:MET:CE	1:C:121:ALA:HB1	2.46	0.45
1:B:108:LEU:HD23	1:B:138:TYR:CG	2.51	0.45
1:A:219:GLN:O	1:A:220:LEU:HG	2.16	0.45
1:A:150:GLU:OE2	1:B:161:ARG:NH2	2.49	0.45
1:A:108:LEU:HD23	1:A:138:TYR:CG	2.51	0.45
1:D:50:ILE:O	1:D:54:VAL:CG1	2.64	0.45
1:D:108:LEU:HD23	1:D:138:TYR:CG	2.51	0.45
1:C:14:ARG:N	1:C:157:GLU:O	2.49	0.45
1:C:237:LYS:HG2	3:C:584:HOH:O	2.17	0.45
1:A:339:PRO:O	1:A:340:ASN:CG	2.54	0.45
1:A:255:VAL:HB	1:A:273:PHE:CZ	2.51	0.45
1:A:73:GLU:HG3	1:A:125:LYS:HZ3	1.82	0.45
1:A:23:LEU:HD22	1:A:48:ASN:OD1	2.16	0.45
1:B:273:PHE:CE1	1:B:345:LEU:HD21	2.52	0.45
1:B:138:TYR:CZ	1:B:142:ARG:HG3	2.52	0.44
1:A:45:VAL:HG22	1:A:125:LYS:HE3	1.98	0.44
1:D:252:ASP:OD1	1:D:276:ASN:ND2	2.46	0.44
1:B:255:VAL:HB	1:B:273:PHE:CZ	2.52	0.44
1:A:220:LEU:CD1	1:A:222:VAL:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ALA:HA	1:C:89:PRO:HB2	1.98	0.44
1:D:14:ARG:HA	1:D:161:ARG:HA	1.99	0.44
1:D:14:ARG:N	1:D:157:GLU:O	2.51	0.44
1:B:262:ASN:HD22	1:B:262:ASN:N	2.14	0.44
1:C:203:ILE:CD1	1:C:237:LYS:O	2.66	0.43
1:B:252:ASP:OD1	1:B:276:ASN:ND2	2.45	0.43
1:C:280:ILE:O	1:C:281:PRO:C	2.54	0.43
1:A:14:ARG:N	1:A:157:GLU:O	2.51	0.43
1:D:220:LEU:HD11	3:D:633:HOH:O	2.18	0.43
1:D:73:GLU:HG3	1:D:74:ARG:HG2	2.00	0.43
1:D:87:GLN:OE1	3:D:503:HOH:O	2.21	0.43
1:B:14:ARG:HA	1:B:161:ARG:HA	2.00	0.43
1:B:14:ARG:N	1:B:157:GLU:O	2.51	0.43
1:B:312:ASP:O	1:B:313:LYS:CB	2.66	0.43
1:A:15:ARG:NH2	1:A:27:TYR:O	2.52	0.43
1:A:61:HIS:CE1	1:A:119:VAL:HG21	2.54	0.43
1:D:183:LYS:HD3	1:D:183:LYS:HA	1.77	0.43
1:C:255:VAL:HB	1:C:273:PHE:CZ	2.54	0.43
1:C:61:HIS:CE1	1:C:119:VAL:HG21	2.53	0.43
1:A:15:ARG:HD3	1:B:144:LYS:HZ1	1.83	0.43
1:B:203:ILE:CD1	1:B:237:LYS:O	2.67	0.43
1:D:39:ALA:HB3	1:D:48:ASN:O	2.19	0.42
1:D:66:LYS:HG3	1:D:84:ARG:O	2.19	0.42
1:C:312:ASP:OD1	1:C:313:LYS:N	2.52	0.42
1:D:255:VAL:HB	1:D:273:PHE:CZ	2.54	0.42
1:B:220:LEU:HD23	1:C:232:THR:HG22	2.01	0.42
1:C:39:ALA:HB1	1:C:43:GLU:CB	2.49	0.42
1:B:316:LEU:HD11	1:B:349:LYS:HE2	2.01	0.42
1:A:124:CYS:HG	2:A:401:TLA:HB	1.65	0.42
1:C:14:ARG:HA	1:C:161:ARG:HA	2.02	0.42
1:D:61:HIS:CE1	1:D:119:VAL:HG21	2.54	0.42
1:B:61:HIS:CE1	1:B:119:VAL:HG21	2.54	0.42
1:B:35:MET:HG3	1:B:123:HIS:HB3	2.02	0.41
1:D:102:LYS:N	1:D:103:PRO:HD2	2.35	0.41
1:C:41:ARG:C	1:C:43:GLU:H	2.24	0.41
1:D:50:ILE:O	1:D:54:VAL:HG12	2.20	0.41
1:B:57:LEU:O	1:B:61:HIS:N	2.47	0.41
1:B:31:ASN:HA	1:B:119:VAL:HG22	2.02	0.41
1:B:74:ARG:NH2	1:B:125:LYS:HE2	2.35	0.41
1:C:14:ARG:HA	1:C:160:THR:O	2.20	0.41
1:D:280:ILE:HD13	1:D:347:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:H	1:C:237:LYS:HG2	1.67	0.41
1:A:150:GLU:CD	1:B:161:ARG:NH1	2.74	0.40
1:A:146:LEU:HB2	1:B:161:ARG:HH12	1.86	0.40
1:D:139:LEU:HD13	1:D:145:PHE:HE2	1.86	0.40
1:B:80:LYS:HE2	1:B:80:LYS:HB2	1.84	0.40
1:D:31:ASN:HA	1:D:119:VAL:HG22	2.03	0.40
1:A:115:ASP:HB3	1:A:118:HIS:CD2	2.56	0.40
1:B:14:ARG:HA	1:B:160:THR:O	2.22	0.40
1:A:72:ALA:HA	1:A:89:PRO:HB2	2.03	0.40
1:D:98:LEU:HD11	1:D:181:LEU:HD11	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:675:HOH:O	3:D:713:HOH:O[6_545]	1.47	0.73
1:C:43:GLU:OE2	1:D:185:HIS:NE2[6_544]	1.83	0.37
1:C:43:GLU:CD	1:D:185:HIS:NE2[6_544]	2.07	0.13

## 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	312/314 (99%)	289 (93%)	20 (6%)	3 (1%)	19	16
1	B	312/314 (99%)	288 (92%)	20 (6%)	4 (1%)	15	11
1	C	312/314 (99%)	289 (93%)	20 (6%)	3 (1%)	19	16
1	D	312/314 (99%)	291 (93%)	19 (6%)	2 (1%)	30	29
All	All	1248/1256 (99%)	1157 (93%)	79 (6%)	12 (1%)	19	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	284	GLU
1	B	45	VAL
1	B	283	PRO
1	B	313	LYS
1	C	46	TYR
1	C	262	ASN
1	C	285	GLU
1	D	284	GLU
1	A	264	MET
1	B	312	ASP
1	D	314	GLU

### 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	273/286 (96%)	266 (97%)	7 (3%)	54	66
1	B	270/286 (94%)	259 (96%)	11 (4%)	37	45
1	C	280/286 (98%)	275 (98%)	5 (2%)	66	79
1	D	280/286 (98%)	269 (96%)	11 (4%)	39	48
All	All	1103/1144 (96%)	1069 (97%)	34 (3%)	47	59

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	142	ARG
1	A	147	LYS
1	A	223	LYS
1	A	229	SER
1	A	284	GLU
1	A	335	ARG
1	B	40	GLU
1	B	41	ARG
1	B	42	LEU

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Mol	Chain	Res	Type
1	B	48	ASN
1	B	60	LYS
1	B	144	LYS
1	B	237	LYS
1	B	262	ASN
1	B	264	MET
1	B	265	LEU
1	B	314	GLU
1	C	74	ARG
1	C	144	LYS
1	C	229	SER
1	C	311	ASN
1	C	335	ARG
1	D	40	GLU
1	D	42	LEU
1	D	54	VAL
1	D	60	LYS
1	D	74	ARG
1	D	125	LYS
1	D	134	MET
1	D	144	LYS
1	D	229	SER
1	D	260	LYS
1	D	269	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	B	48	ASN
1	B	262	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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	$\# Z  > 2$
2	TLA	A	401	-	3,9,9	0.21	0	6,12,12	1.18	0
2	TLA	B	401	-	3,9,9	0.44	0	6,12,12	1.25	1 (16%)
2	TLA	C	401	-	3,9,9	0.42	0	6,12,12	1.36	1 (16%)
2	TLA	D	401	-	3,9,9	0.43	0	6,12,12	1.52	1 (16%)

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
2	TLA	A	401	-	-	0/4/12/12	0/0/0/0
2	TLA	B	401	-	-	0/4/12/12	0/0/0/0
2	TLA	C	401	-	-	0/4/12/12	0/0/0/0
2	TLA	D	401	-	-	0/4/12/12	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	TLA	C1-C2-C3	-3.09	107.02	113.35
2	C	401	TLA	C1-C2-C3	-2.49	108.24	113.35
2	B	401	TLA	C1-C2-C3	-2.25	108.73	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TLA	2	0
2	B	401	TLA	1	0
2	C	401	TLA	1	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	314/314 (100%)	-0.02	14 (4%) 37 36	37, 53, 94, 115	1 (0%)
1	B	314/314 (100%)	0.16	24 (7%) 17 16	38, 56, 107, 135	2 (0%)
1	C	314/314 (100%)	-0.04	6 (1%) 70 68	39, 54, 97, 124	0
1	D	314/314 (100%)	0.05	9 (2%) 55 54	39, 56, 101, 118	0
All	All	1256/1256 (100%)	0.04	53 (4%) 40 39	37, 55, 101, 135	3 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	PRO	7.2
1	D	265	LEU	5.2
1	B	44	GLY	5.1
1	B	265	LEU	5.1
1	A	311	ASN	5.0
1	D	40	GLU	4.5
1	B	284	GLU	4.5
1	A	44	GLY	4.4
1	B	46	TYR	4.1
1	A	282	GLY	4.0
1	B	40	GLU	4.0
1	B	262	ASN	3.8
1	A	265	LEU	3.6
1	B	81	PHE	3.5
1	B	264	MET	3.4
1	C	264	MET	3.4
1	D	76	TYR	3.4
1	A	261	GLN	3.3
1	A	283	PRO	3.2
1	B	47	ARG	3.2
1	C	45	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	285	GLU	3.0
1	B	82	ASN	3.0
1	C	265	LEU	2.8
1	D	42	LEU	2.8
1	B	43	GLU	2.7
1	D	283	PRO	2.7
1	B	261	GLN	2.6
1	D	50	ILE	2.6
1	A	262	ASN	2.6
1	A	45	VAL	2.6
1	B	45	VAL	2.6
1	D	79	ALA	2.5
1	C	261	GLN	2.5
1	A	42	LEU	2.5
1	A	310	ASP	2.5
1	B	37	PHE	2.4
1	C	79	ALA	2.4
1	A	264	MET	2.4
1	A	43	GLU	2.3
1	B	186	LEU	2.3
1	B	263	LYS	2.3
1	B	311	ASN	2.3
1	A	268	ASP	2.3
1	B	266	LYS	2.3
1	B	42	LEU	2.3
1	B	14	ARG	2.3
1	C	266	LYS	2.3
1	B	312	ASP	2.2
1	B	267	LYS	2.1
1	D	46	TYR	2.1
1	A	285	GLU	2.1
1	D	41	ARG	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TLA	D	401	10/10	0.95	0.14	0.92	58,63,71,72	0
2	TLA	B	401	10/10	0.94	0.14	0.19	56,63,78,82	0
2	TLA	C	401	10/10	0.95	0.12	-0.37	55,57,61,63	0
2	TLA	A	401	10/10	0.94	0.11	-0.78	50,55,58,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.