



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:17 PM GMT

PDB ID : 4QN9  
Title : Structure of human NAPE-PLD  
Authors : Garau, G.  
Deposited on : 2014-06-17  
Resolution : 2.65 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

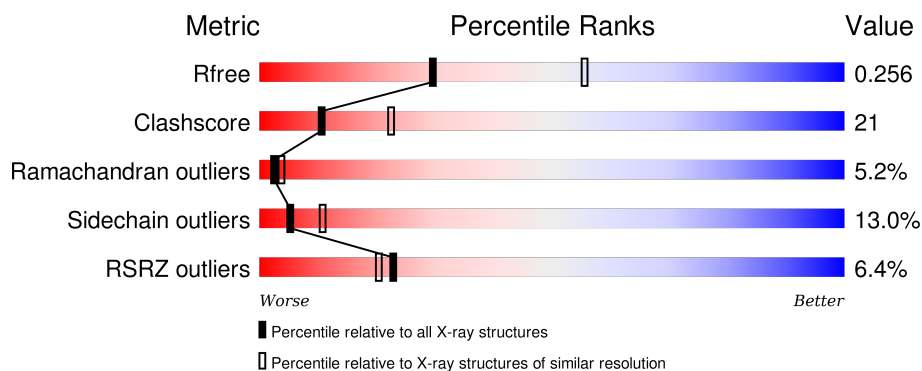
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	393	<div> <div>7%</div> <div>53%</div> <div>19%</div> <div>7%</div> <div>•</div> <div>18%</div> </div>
1	B	393	<div> <div>4%</div> <div>52%</div> <div>21%</div> <div>7%</div> <div>•</div> <div>18%</div> </div>

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
2	ZN	B	604	-	-	-	X
4	DXC	B	608	-	-	-	X
4	DXC	B	609	-	-	-	X
4	DXC	B	610	-	-	-	X
5	SO4	B	611	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5875 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.

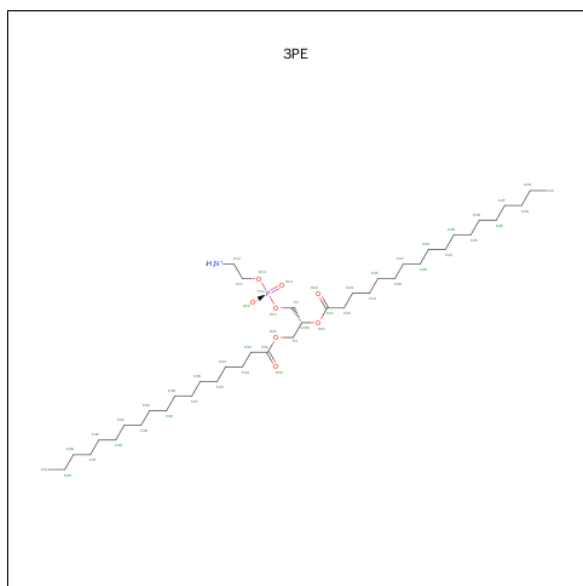
- Molecule 1 is a protein called N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	8	0
			2679	1732	452	482	13			
1	B	322	Total	C	N	O	S	0	7	0
			2682	1732	452	485	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

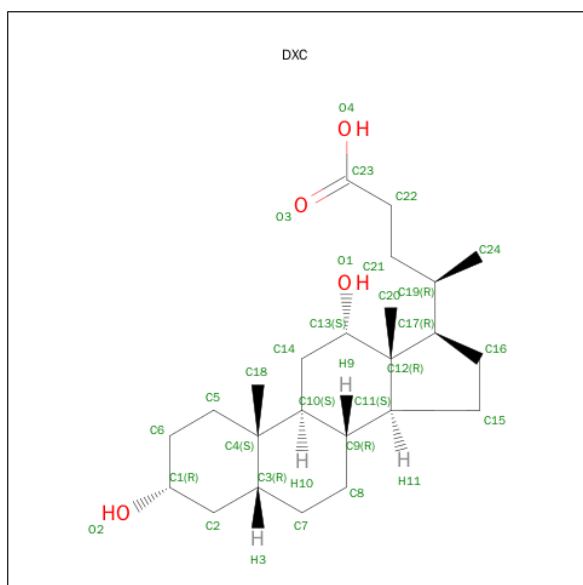
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

- Molecule 4 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	A	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			28	24	4		
4	B	1	Total	C	O	0	0
			28	24	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

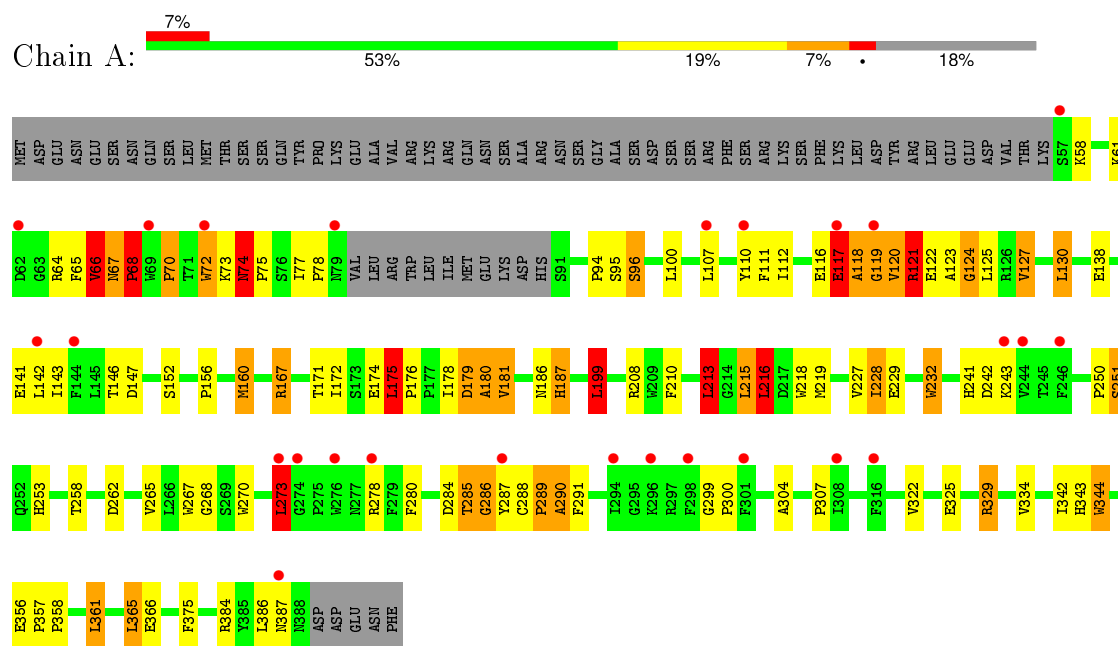
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	62	Total	O	0	1
			63	63		

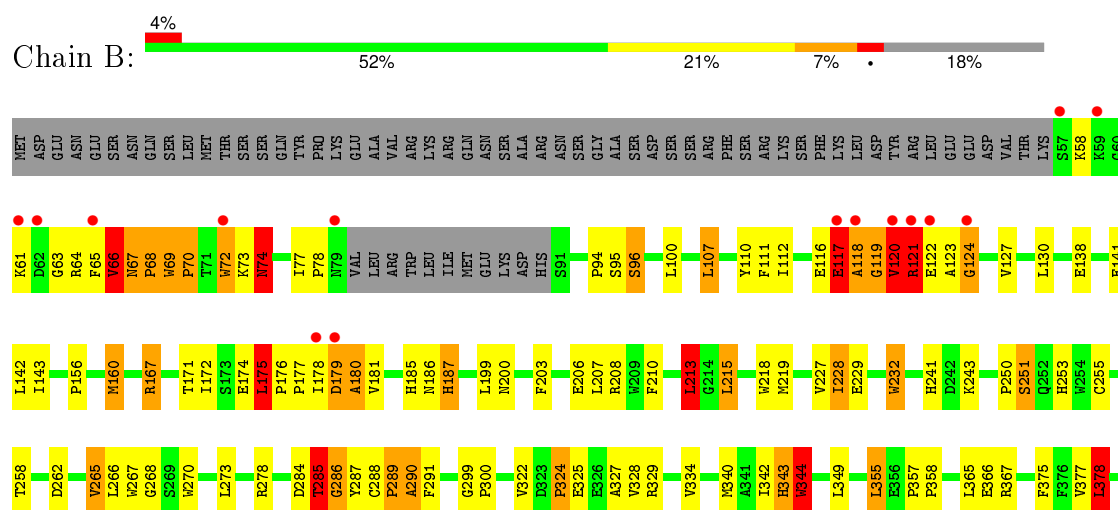
### 3 Residue-property plots

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: N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D



- Molecule 1: N-acyl-phosphatidylethanolamine-hydrolyzing phospholipase D



1386			
1387			
1388			
1389			
ASP			
GLU			
ASN			
PHE			



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.10 Å 95.10 Å 444.17 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.36 – 2.65 82.36 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (82.36-2.65) 100.0 (82.36-2.65)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.65 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.214 , 0.253 0.217 , 0.256	Depositor DCC
$R_{free}$ test set	1794 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35841 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DXC, SO4, 3PE

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	1/2774 (0.0%)	1.12	25/3777 (0.7%)
1	B	0.83	2/2773 (0.1%)	1.13	25/3777 (0.7%)
All	All	0.75	3/5547 (0.1%)	1.13	50/7554 (0.7%)

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	9
1	B	0	8
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	TRP	CB-CG	8.52	1.65	1.50
1	A	72	TRP	CB-CG	6.10	1.61	1.50
1	B	69	TRP	CB-CG	-5.59	1.40	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-22.64	108.98	120.30
1	B	121	ARG	NE-CZ-NH1	-16.39	112.10	120.30
1	B	121	ARG	NE-CZ-NH2	13.98	127.29	120.30
1	A	121	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	A	121	ARG	CD-NE-CZ	10.84	138.77	123.60
1	B	384	ARG	NE-CZ-NH2	-8.30	116.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ARG	CD-NE-CZ	7.20	133.69	123.60
1	B	232	TRP	CA-CB-CG	7.11	127.21	113.70
1	A	232	TRP	CA-CB-CG	6.80	126.61	113.70
1	A	287	TYR	N-CA-C	-6.79	92.67	111.00
1	B	175[A]	LEU	CA-CB-CG	6.68	130.66	115.30
1	B	175[B]	LEU	CA-CB-CG	6.68	130.66	115.30
1	A	361	LEU	CB-CG-CD2	6.41	121.90	111.00
1	B	328	VAL	CG1-CB-CG2	6.37	121.08	110.90
1	B	175[A]	LEU	C-N-CD	-6.30	106.73	120.60
1	B	175[B]	LEU	C-N-CD	-6.30	106.73	120.60
1	B	384	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	213	LEU	CB-CG-CD2	6.22	121.57	111.00
1	A	329	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	A	127	VAL	CG1-CB-CG2	6.16	120.75	110.90
1	A	215	LEU	CB-CG-CD2	6.16	121.47	111.00
1	B	215	LEU	CB-CG-CD1	6.07	121.32	111.00
1	B	142	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	273	LEU	CB-CG-CD2	5.91	121.04	111.00
1	B	287	TYR	N-CA-C	-5.89	95.09	111.00
1	A	365	LEU	CB-CG-CD1	5.89	121.01	111.00
1	A	66	VAL	CG1-CB-CG2	5.84	120.25	110.90
1	A	130	LEU	CB-CG-CD1	5.84	120.92	111.00
1	A	199	LEU	CB-CG-CD1	5.77	120.81	111.00
1	A	175[A]	LEU	CA-CB-CG	5.69	128.40	115.30
1	A	175[B]	LEU	CA-CB-CG	5.69	128.40	115.30
1	B	378	LEU	CB-CG-CD1	5.68	120.66	111.00
1	A	107	LEU	CB-CG-CD2	5.65	120.60	111.00
1	B	107	LEU	CB-CG-CD1	5.58	120.48	111.00
1	A	213	LEU	CB-CG-CD1	5.56	120.46	111.00
1	A	142	LEU	CB-CG-CD2	5.55	120.44	111.00
1	B	130	LEU	CB-CG-CD2	5.39	120.16	111.00
1	A	265	VAL	CG1-CB-CG2	5.37	119.50	110.90
1	B	365	LEU	CB-CG-CD2	5.34	120.08	111.00
1	B	66	VAL	CG1-CB-CG2	5.33	119.43	110.90
1	A	216	LEU	CB-CG-CD1	5.31	120.03	111.00
1	B	355	LEU	CB-CG-CD1	5.31	120.02	111.00
1	A	216	LEU	CB-CG-CD2	5.30	120.01	111.00
1	A	181	VAL	CG1-CB-CG2	5.27	119.33	110.90
1	B	265	VAL	CG1-CB-CG2	5.15	119.13	110.90
1	A	175[A]	LEU	C-N-CD	-5.12	109.34	120.60
1	A	175[B]	LEU	C-N-CD	-5.12	109.34	120.60
1	B	175[A]	LEU	CB-CG-CD2	5.11	119.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175[B]	LEU	CB-CG-CD2	5.11	119.68	111.00
1	B	285	THR	C-N-CA	-5.03	111.73	122.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	GLU	Peptide
1	A	117	GLU	Peptide
1	A	118	ALA	Peptide
1	A	121	ARG	Sidechain
1	A	175[A]	LEU	Peptide
1	A	285	THR	Mainchain,Peptide
1	A	286	GLY	Mainchain,Peptide
1	B	116	GLU	Peptide
1	B	117	GLU	Peptide
1	B	118	ALA	Peptide
1	B	120	VAL	Peptide
1	B	175[A]	LEU	Peptide
1	B	285	THR	Peptide
1	B	286	GLY	Mainchain,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	2679	0	2572	94	0
1	B	2682	0	2567	108	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	62	1	0
3	B	44	0	62	1	0
4	A	112	0	156	18	0
4	B	196	0	273	34	0
5	A	10	0	0	1	0
5	B	5	0	0	2	0
6	A	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	63	0	0	3	0
All	All	5875	0	5692	244	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 21.

All (244) 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:B:118:ALA:HB1	1:B:138:GLU:OE1	1.41	1.17
4:B:610:DXC:H203	4:B:610:DXC:H242	1.19	1.14
1:A:118:ALA:HB1	1:A:138:GLU:OE1	1.50	1.10
1:B:175[B]:LEU:HB2	1:B:176[B]:PRO:HD2	1.09	1.07
1:A:232:TRP:HZ3	1:A:267:TRP:O	1.39	1.06
1:B:232:TRP:HZ3	1:B:267:TRP:O	1.39	1.05
1:B:175[B]:LEU:CB	1:B:176[B]:PRO:HD2	1.84	1.03
1:A:175[B]:LEU:CB	1:A:176[B]:PRO:HD2	1.83	1.03
1:A:175[B]:LEU:HD12	1:A:175[B]:LEU:H	1.25	1.00
1:A:175[B]:LEU:HB2	1:A:176[B]:PRO:HD2	1.39	0.99
1:B:175[B]:LEU:H	1:B:175[B]:LEU:HD22	1.30	0.92
1:B:175[B]:LEU:HB2	1:B:176[B]:PRO:CD	1.97	0.91
1:B:65:PHE:O	1:B:66:VAL:HB	1.71	0.90
1:B:174[A]:GLU:O	1:B:175[A]:LEU:HG	1.72	0.89
1:A:143:ILE:O	1:A:179[B]:ASP:HB3	1.75	0.87
1:B:286:GLY:HA2	1:B:322:VAL:HG13	1.54	0.86
1:A:232:TRP:CZ3	1:A:267:TRP:O	2.27	0.85
1:B:175[B]:LEU:CD2	1:B:175[B]:LEU:H	1.89	0.85
1:A:178[B]:ILE:HA	1:A:179[B]:ASP:HB2	1.58	0.85
1:B:186:ASN:O	1:B:187:HIS:HB2	1.76	0.85
1:B:119:GLY:HA3	1:B:138:GLU:HB3	1.57	0.84
1:B:118:ALA:CB	1:B:138:GLU:OE1	2.26	0.84
1:B:232:TRP:CZ3	1:B:267:TRP:O	2.29	0.84
4:B:603:DXC:H221	4:B:603:DXC:H161	1.62	0.81
1:A:174[A]:GLU:O	1:A:175[A]:LEU:HB2	1.80	0.81
1:A:175[B]:LEU:CB	1:A:176[B]:PRO:CD	2.59	0.80
1:A:67:ASN:HB2	1:A:68:PRO:HD2	1.61	0.80
1:A:289:PRO:O	1:A:290:ALA:HB3	1.82	0.80
1:B:143:ILE:O	1:B:179[B]:ASP:HB3	1.82	0.80
1:A:186:ASN:O	1:A:187:HIS:HB2	1.80	0.79
1:B:178[B]:ILE:HA	1:B:179[B]:ASP:HB2	1.66	0.78
4:B:610:DXC:H242	4:B:610:DXC:C20	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG22	1:A:141:GLU:HA	1.65	0.77
1:B:66:VAL:O	1:B:67:ASN:CG	2.24	0.77
1:A:118:ALA:CB	1:A:138:GLU:OE1	2.33	0.76
1:B:175[B]:LEU:CB	1:B:176[B]:PRO:CD	2.60	0.75
1:B:66:VAL:O	1:B:67:ASN:CB	2.35	0.74
1:B:69:TRP:HH2	1:B:213:LEU:HD13	1.52	0.74
1:B:171:THR:HG1	1:B:174[B]:GLU:HG3	1.52	0.73
1:A:66:VAL:O	1:A:67:ASN:CG	2.27	0.73
1:B:120:VAL:HG22	1:B:141:GLU:HA	1.70	0.72
1:A:174[A]:GLU:O	1:A:175[A]:LEU:CB	2.38	0.72
1:B:289:PRO:O	1:B:290:ALA:HB3	1.89	0.71
1:A:171:THR:HG1	1:A:174[B]:GLU:HG3	1.54	0.70
1:B:179[B]:ASP:O	1:B:180[B]:ALA:HB2	1.91	0.70
1:B:67:ASN:HB2	1:B:68:PRO:HD2	1.71	0.70
4:A:507:DXC:H221	4:A:507:DXC:H161	1.72	0.69
1:B:167:ARG:NH2	5:B:611:SO4:O3	2.26	0.69
1:A:286:GLY:HA2	1:A:322:VAL:HG13	1.75	0.69
1:A:119:GLY:HA2	1:A:138:GLU:HB3	1.74	0.68
1:A:160:MET:HE1	4:A:505:DXC:H243	1.76	0.68
4:B:610:DXC:H241	4:B:610:DXC:H13	1.75	0.68
1:A:179[B]:ASP:O	1:A:180[B]:ALA:HB2	1.93	0.68
1:A:160:MET:CE	4:A:505:DXC:H243	2.25	0.67
1:A:289:PRO:O	1:A:290:ALA:CB	2.42	0.67
1:A:175[B]:LEU:N	1:A:175[B]:LEU:HD12	2.03	0.67
4:B:610:DXC:H203	4:B:610:DXC:C24	2.08	0.66
1:A:66:VAL:O	1:A:67:ASN:CB	2.41	0.66
1:A:178[B]:ILE:CA	1:A:179[B]:ASP:HB2	2.25	0.66
1:B:66:VAL:O	1:B:67:ASN:ND2	2.29	0.66
1:B:174[A]:GLU:O	1:B:175[A]:LEU:CB	2.43	0.65
1:B:218:TRP:CE3	1:B:219:MET:HE2	2.31	0.65
1:B:186:ASN:O	1:B:187:HIS:CB	2.42	0.64
1:B:119:GLY:CA	1:B:138:GLU:HB3	2.26	0.64
4:B:608:DXC:H242	4:B:608:DXC:H13	1.80	0.63
1:A:175[B]:LEU:HB3	1:A:176[B]:PRO:HD2	1.79	0.63
1:A:67:ASN:CB	1:A:68:PRO:HD2	2.27	0.62
1:B:218:TRP:HE3	1:B:219:MET:HE2	1.64	0.62
1:B:175[B]:LEU:CD2	1:B:175[B]:LEU:N	2.61	0.62
1:A:119:GLY:CA	1:A:138:GLU:HB3	2.29	0.62
1:A:186:ASN:O	1:A:187:HIS:CB	2.47	0.62
1:A:213:LEU:HA	1:A:229:GLU:HG2	1.82	0.61
1:A:167:ARG:HH21	1:A:167:ARG:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASN:O	1:B:203:PHE:O	2.18	0.61
1:A:66:VAL:HG23	1:A:66:VAL:O	2.01	0.61
1:A:218:TRP:HE3	1:A:219:MET:HE2	1.65	0.60
1:A:288:CYS:C	1:A:289:PRO:O	2.39	0.60
1:B:289:PRO:O	1:B:290:ALA:CB	2.46	0.60
1:A:218:TRP:CE3	1:A:219:MET:HE2	2.37	0.60
1:B:66:VAL:O	1:B:66:VAL:HG13	2.02	0.59
1:A:66:VAL:O	1:A:67:ASN:ND2	2.35	0.59
1:B:288:CYS:C	1:B:289:PRO:O	2.41	0.59
4:B:610:DXC:H13	4:B:610:DXC:C24	2.32	0.58
1:B:178[B]:ILE:CA	1:B:179[B]:ASP:HB2	2.32	0.58
1:B:218:TRP:CE3	1:B:219:MET:CE	2.86	0.58
1:B:167:ARG:HB3	1:B:167:ARG:HH21	1.68	0.58
4:B:609:DXC:H183	4:B:610:DXC:H181	1.86	0.58
1:A:299:GLY:HA2	1:A:300:PRO:C	2.23	0.58
1:A:167:ARG:NH2	5:A:508:SO4:O1	2.33	0.58
1:B:213:LEU:HA	1:B:229:GLU:HG2	1.84	0.57
1:B:67:ASN:CB	1:B:68:PRO:HD2	2.34	0.57
1:B:69:TRP:CH2	1:B:213:LEU:HD13	2.37	0.57
1:B:118:ALA:HB3	6:B:710:HOH:O	2.04	0.57
1:B:174[A]:GLU:O	1:B:175[A]:LEU:CG	2.50	0.57
1:B:120:VAL:O	1:B:121:ARG:HB2	2.05	0.56
1:B:123:ALA:O	1:B:124:GLY:O	2.23	0.56
1:A:67:ASN:HB2	1:A:68:PRO:CD	2.33	0.56
1:A:65:PHE:O	1:A:66:VAL:HG22	2.06	0.55
1:A:172:ILE:HG23	1:A:199:LEU:HD13	1.88	0.55
4:A:505:DXC:H242	4:A:505:DXC:H13	1.87	0.55
4:A:504:DXC:H243	1:B:160:MET:HE1	1.89	0.55
4:B:603:DXC:C22	4:B:603:DXC:H161	2.36	0.54
1:A:286:GLY:CA	1:A:322:VAL:HG13	2.37	0.54
1:B:179[B]:ASP:O	1:B:180[B]:ALA:CB	2.55	0.54
1:B:66:VAL:O	1:B:67:ASN:HB3	2.07	0.54
1:B:210:PHE:HB3	1:B:270:TRP:CH2	2.42	0.54
1:B:388:ASN:O	1:B:389:ASP:HB2	2.07	0.54
4:A:504:DXC:H13	4:A:504:DXC:H242	1.89	0.53
1:B:299:GLY:HA2	1:B:300:PRO:C	2.28	0.53
4:B:603:DXC:C13	4:B:603:DXC:H242	2.39	0.53
1:A:210:PHE:HB3	1:A:270:TRP:CH2	2.42	0.53
1:B:120:VAL:CG1	1:B:122:GLU:OE2	2.56	0.53
1:B:179[A]:ASP:HB3	1:B:206:GLU:O	2.08	0.53
1:A:171:THR:OG1	1:A:174[A]:GLU:OE1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:504:DXC:H243	1:B:160:MET:CE	2.37	0.53
1:B:66:VAL:O	1:B:66:VAL:CG1	2.56	0.53
1:A:179[B]:ASP:O	1:A:180[B]:ALA:CB	2.57	0.52
1:B:251:SER:HB3	1:B:268:GLY:HA2	1.92	0.52
1:B:227:VAL:O	1:B:228:ILE:HD12	2.08	0.52
1:B:178[B]:ILE:HG22	1:B:180[B]:ALA:H	1.75	0.52
4:A:507:DXC:H161	4:A:507:DXC:C22	2.39	0.52
4:B:603:DXC:C22	4:B:603:DXC:C16	2.89	0.51
4:A:507:DXC:C13	4:A:507:DXC:H242	2.41	0.51
4:B:603:DXC:H221	4:B:603:DXC:C16	2.37	0.51
4:A:507:DXC:H182	4:B:607:DXC:H203	1.92	0.51
1:A:120:VAL:HG12	1:A:121:ARG:H	1.74	0.51
4:B:609:DXC:C24	4:B:609:DXC:C13	2.89	0.51
1:A:258:THR:HG21	4:A:507:DXC:H3	1.92	0.51
1:A:120:VAL:O	1:A:121:ARG:HB2	2.10	0.50
1:B:357:PRO:HB2	1:B:358:PRO:HD3	1.93	0.50
4:B:609:DXC:H241	4:B:609:DXC:O1	2.10	0.50
1:B:64:ARG:HA	1:B:70:PRO:HD3	1.93	0.50
1:B:384:ARG:HD3	6:B:750:HOH:O	2.11	0.50
1:B:120:VAL:HG12	1:B:122:GLU:OE2	2.11	0.50
1:A:64:ARG:HA	1:A:70:PRO:HD3	1.94	0.49
1:B:120:VAL:HG12	1:B:121:ARG:N	2.28	0.49
4:B:609:DXC:H242	4:B:609:DXC:C13	2.42	0.49
4:B:601:DXC:H203	4:B:603:DXC:H182	1.94	0.49
1:A:285:THR:HG21	1:A:291:PHE:CZ	2.47	0.49
1:A:120:VAL:HG12	1:A:121:ARG:N	2.27	0.49
1:A:179[A]:ASP:O	1:A:208:ARG:N	2.27	0.49
1:B:63:GLY:O	1:B:70:PRO:HD2	2.13	0.49
1:B:175[A]:LEU:HB3	1:B:177[A]:PRO:HD3	1.95	0.48
1:B:120:VAL:HG12	1:B:121:ARG:H	1.78	0.48
1:A:175[B]:LEU:H	1:A:175[B]:LEU:CD1	2.03	0.48
1:A:178[B]:ILE:HG22	1:A:180[B]:ALA:H	1.79	0.48
4:B:609:DXC:H242	4:B:609:DXC:H13	1.96	0.47
1:B:273:LEU:HD22	1:B:278:ARG:HD2	1.97	0.47
1:A:119:GLY:C	1:A:120:VAL:HG23	2.35	0.47
4:B:607:DXC:H13	4:B:607:DXC:H242	1.95	0.47
1:A:218:TRP:CE3	1:A:219:MET:CE	2.97	0.47
1:A:167:ARG:NH2	1:B:171:THR:HG21	2.29	0.47
4:B:603:DXC:H242	4:B:603:DXC:O1	2.14	0.47
1:B:174[A]:GLU:OE1	1:B:174[A]:GLU:N	2.48	0.47
1:A:232:TRP:CE3	1:A:250:PRO:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:OG1	1:B:174[A]:GLU:OE1	2.28	0.47
1:A:175[B]:LEU:HB2	1:A:176[B]:PRO:CD	2.20	0.47
4:B:601:DXC:H242	4:B:601:DXC:H13	1.96	0.47
1:B:285:THR:HG21	1:B:291:PHE:CZ	2.50	0.47
4:B:603:DXC:H71	4:B:603:DXC:H182	1.60	0.47
4:B:610:DXC:C13	4:B:610:DXC:C24	2.93	0.46
1:B:67:ASN:HB2	1:B:68:PRO:CD	2.43	0.46
4:B:603:DXC:H61	4:B:603:DXC:H10	1.74	0.46
1:B:340:MET:SD	1:B:378:LEU:HD22	2.55	0.46
1:B:180[A]:ALA:HA	1:B:208:ARG:O	2.14	0.46
1:B:172:ILE:O	1:B:175[B]:LEU:CD2	2.63	0.46
1:B:258:THR:HG21	4:B:603:DXC:H3	1.97	0.46
1:A:120:VAL:CG1	1:A:122:GLU:OE2	2.64	0.46
4:A:507:DXC:H182	4:A:507:DXC:H71	1.60	0.46
1:A:110:TYR:OH	1:A:118:ALA:CB	2.64	0.46
1:B:68:PRO:HD3	6:B:758:HOH:O	2.15	0.46
1:A:156:PRO:HD2	3:A:503:3PE:H362	1.98	0.45
1:A:67:ASN:CB	1:A:68:PRO:CD	2.92	0.45
4:A:507:DXC:C16	4:A:507:DXC:C22	2.94	0.45
1:A:120:VAL:HG12	1:A:122:GLU:OE2	2.17	0.45
4:A:507:DXC:H61	4:A:507:DXC:H10	1.74	0.45
1:A:111:PHE:CD2	1:A:175[B]:LEU:HA	2.52	0.45
1:A:125:LEU:HD23	1:A:125:LEU:C	2.38	0.44
1:B:94:PRO:O	1:B:95:SER:HB2	2.16	0.44
4:A:507:DXC:C8	4:B:602:DXC:H222	2.48	0.44
4:B:608:DXC:C24	4:B:608:DXC:H13	2.47	0.44
1:B:111:PHE:CD2	1:B:175[B]:LEU:HA	2.52	0.44
1:A:167:ARG:HH21	1:A:167:ARG:CB	2.31	0.44
1:A:172:ILE:HA	1:A:175[B]:LEU:HD11	1.99	0.44
1:A:227:VAL:O	1:A:228:ILE:HD12	2.18	0.44
1:A:180[A]:ALA:HA	1:A:208:ARG:O	2.18	0.43
1:A:66:VAL:O	1:A:67:ASN:HB3	2.14	0.43
1:A:253:HIS:CE1	1:A:284:ASP:HB3	2.52	0.43
4:B:603:DXC:H201	4:B:603:DXC:H9	1.53	0.43
1:B:185:HIS:HB2	1:B:255:CYS:SG	2.58	0.43
4:A:507:DXC:H9	4:A:507:DXC:H201	1.52	0.43
1:B:118:ALA:HA	1:B:121:ARG:NH1	2.32	0.43
1:B:218:TRP:CZ3	1:B:219:MET:CE	3.01	0.43
1:A:357:PRO:HB2	1:A:358:PRO:HD3	2.00	0.43
1:B:112:ILE:HG12	1:B:174[A]:GLU:HG2	2.01	0.43
1:A:288:CYS:HG	1:A:290:ALA:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178[A]:ILE:HA	1:B:179[A]:ASP:HA	1.72	0.42
1:A:216:LEU:HB2	1:A:229:GLU:CD	2.40	0.42
1:B:215:LEU:HD13	1:B:265:VAL:HG11	2.02	0.42
1:A:178[A]:ILE:HA	1:A:179[A]:ASP:HA	1.73	0.42
1:A:112:ILE:HG12	1:A:174[A]:GLU:HG2	2.00	0.42
1:A:280:PHE:O	1:A:304:ALA:HA	2.19	0.42
1:B:174[A]:GLU:O	1:B:175[A]:LEU:HB2	2.19	0.42
1:A:123:ALA:O	1:A:124:GLY:O	2.36	0.42
1:B:119:GLY:C	1:B:120:VAL:HG23	2.40	0.42
1:A:288:CYS:SG	1:A:289:PRO:O	2.77	0.42
1:B:172:ILE:HD13	1:B:199:LEU:HG	2.02	0.42
1:A:174[A]:GLU:N	1:A:174[A]:GLU:OE1	2.52	0.42
4:A:507:DXC:O1	4:A:507:DXC:H242	2.19	0.42
1:B:253:HIS:CE1	1:B:284:ASP:HB3	2.55	0.42
1:B:232:TRP:CE3	1:B:250:PRO:HA	2.55	0.42
1:A:172:ILE:O	1:A:175[B]:LEU:CD1	2.68	0.42
1:B:273:LEU:HD22	1:B:278:ARG:CD	2.50	0.42
1:B:74:ASN:OD1	1:B:74:ASN:N	2.52	0.42
4:B:610:DXC:H222	4:B:610:DXC:H243	1.71	0.42
1:B:156:PRO:HD2	3:B:606:3PE:H362	2.00	0.42
1:B:232:TRP:CZ3	1:B:266:LEU:HD22	2.55	0.41
1:A:356:GLU:N	1:A:357:PRO:CD	2.83	0.41
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.93	0.41
4:B:609:DXC:H242	4:B:609:DXC:H203	2.03	0.41
1:B:181:VAL:HG23	1:B:207:LEU:HD11	2.02	0.41
4:B:609:DXC:C24	4:B:609:DXC:O1	2.68	0.41
1:A:117:GLU:HB2	1:A:121:ARG:NH2	2.36	0.41
1:A:94:PRO:O	1:A:95:SER:HB2	2.20	0.41
1:A:74:ASN:N	1:A:75:PRO:HD2	2.35	0.41
1:A:307:PRO:HA	1:A:342:ILE:O	2.20	0.41
1:A:251:SER:HB3	1:A:268:GLY:HA2	2.01	0.41
1:A:77:ILE:HG22	1:A:78:PRO:HD2	2.02	0.41
1:B:171:THR:OG1	1:B:174[B]:GLU:HG3	2.18	0.41
4:A:507:DXC:H82	4:B:602:DXC:H222	2.01	0.41
1:B:77:ILE:HG22	1:B:78:PRO:HD2	2.02	0.41
1:B:324:PRO:O	1:B:327:ALA:HB3	2.20	0.41
1:B:175[B]:LEU:HD22	1:B:175[B]:LEU:N	2.14	0.41
1:B:65:PHE:O	1:B:66:VAL:CB	2.55	0.41
1:A:178[B]:ILE:HA	1:A:179[B]:ASP:CB	2.41	0.41
4:B:607:DXC:H201	4:B:607:DXC:H142	1.82	0.41
1:B:110:TYR:OH	1:B:118:ALA:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:O	1:A:147:ASP:C	2.59	0.40
1:B:342:ILE:C	1:B:343:HIS:O	2.58	0.40
1:B:167:ARG:NH1	5:B:611:SO4:O3	2.54	0.40
1:B:177[A]:PRO:HD2	1:B:203:PHE:CZ	2.56	0.40
1:A:273:LEU:HD12	1:A:278:ARG:HD2	2.03	0.40
4:B:609:DXC:H182	4:B:609:DXC:H9	1.91	0.40
1:B:343:HIS:O	1:B:344:TRP:CD1	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/393 (83%)	284 (87%)	22 (7%)	19 (6%)	2	3
1	B	325/393 (83%)	281 (86%)	26 (8%)	18 (6%)	2	3
All	All	650/786 (83%)	565 (87%)	48 (7%)	37 (6%)	2	3

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	67	ASN
1	A	119	GLY
1	A	120	VAL
1	A	121	ARG
1	A	187	HIS
1	B	66	VAL
1	B	67	ASN
1	B	119	GLY
1	B	120	VAL
1	B	121	ARG

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Mol	Chain	Res	Type
1	B	187	HIS
1	A	117	GLU
1	A	124	GLY
1	A	179[A]	ASP
1	A	179[B]	ASP
1	A	344	TRP
1	B	117	GLU
1	B	124	GLY
1	B	179[A]	ASP
1	B	179[B]	ASP
1	B	180[A]	ALA
1	B	180[B]	ALA
1	B	290	ALA
1	B	344	TRP
1	A	70	PRO
1	A	180[A]	ALA
1	A	180[B]	ALA
1	A	290	ALA
1	B	70	PRO
1	A	289	PRO
1	B	96	SER
1	A	68	PRO
1	A	96	SER
1	B	289	PRO
1	B	74	ASN
1	A	74	ASN

### 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	291/352 (83%)	250 (86%)	41 (14%)	4	8
1	B	291/352 (83%)	257 (88%)	34 (12%)	7	13
All	All	582/704 (83%)	507 (87%)	75 (13%)	5	11

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	61	LYS
1	A	66	VAL
1	A	68	PRO
1	A	72	TRP
1	A	73	LYS
1	A	74	ASN
1	A	96	SER
1	A	100	LEU
1	A	117	GLU
1	A	127	VAL
1	A	130	LEU
1	A	152	SER
1	A	160	MET
1	A	167	ARG
1	A	175[A]	LEU
1	A	175[B]	LEU
1	A	181	VAL
1	A	199	LEU
1	A	213	LEU
1	A	215	LEU
1	A	216	LEU
1	A	228	ILE
1	A	241	HIS
1	A	242	ASP
1	A	243	LYS
1	A	251	SER
1	A	262	ASP
1	A	273	LEU
1	A	325	GLU
1	A	329	ARG
1	A	334	VAL
1	A	343	HIS
1	A	344	TRP
1	A	361	LEU
1	A	365	LEU
1	A	366	GLU
1	A	375	PHE
1	A	384	ARG
1	A	386	LEU
1	A	387	ASN
1	B	58	LYS
1	B	61	LYS

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Mol	Chain	Res	Type
1	B	66	VAL
1	B	68	PRO
1	B	72	TRP
1	B	73	LYS
1	B	74	ASN
1	B	96	SER
1	B	107	LEU
1	B	117	GLU
1	B	127	VAL
1	B	160	MET
1	B	167	ARG
1	B	213	LEU
1	B	228	ILE
1	B	241	HIS
1	B	243	LYS
1	B	251	SER
1	B	262	ASP
1	B	324	PRO
1	B	325	GLU
1	B	329	ARG
1	B	334	VAL
1	B	343	HIS
1	B	344	TRP
1	B	349	LEU
1	B	355	LEU
1	B	366	GLU
1	B	367	ARG
1	B	375	PHE
1	B	377	VAL
1	B	378	LEU
1	B	384	ARG
1	B	387	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	B	277	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 ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	3PE	A	503	2	43,43,50	0.96	3 (6%)	45,48,55	1.41	4 (8%)
4	DXC	A	504	-	28,31,31	0.85	2 (7%)	46,49,49	1.41	9 (19%)
4	DXC	A	505	-	28,31,31	0.89	1 (3%)	46,49,49	1.39	8 (17%)
4	DXC	A	506	-	28,31,31	0.87	1 (3%)	46,49,49	1.32	6 (13%)
4	DXC	A	507	-	28,31,31	1.20	3 (10%)	46,49,49	3.52	21 (45%)
5	SO4	A	508	-	4,4,4	0.47	0	6,6,6	0.36	0
5	SO4	A	509	-	4,4,4	0.62	0	6,6,6	0.22	0
4	DXC	B	601	-	28,31,31	0.93	1 (3%)	46,49,49	1.37	8 (17%)
4	DXC	B	602	-	28,31,31	0.88	1 (3%)	46,49,49	1.21	4 (8%)
4	DXC	B	603	-	28,31,31	1.27	1 (3%)	46,49,49	3.85	22 (47%)
3	3PE	B	606	2	43,43,50	1.01	2 (4%)	45,48,55	1.44	6 (13%)
4	DXC	B	607	-	28,31,31	1.07	3 (10%)	46,49,49	1.52	9 (19%)
4	DXC	B	608	-	28,31,31	1.10	3 (10%)	46,49,49	1.59	10 (21%)
4	DXC	B	609	-	28,31,31	1.13	3 (10%)	46,49,49	2.14	13 (28%)
4	DXC	B	610	-	28,31,31	0.91	2 (7%)	46,49,49	2.45	18 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	611	-	4,4,4	0.76	0	6,6,6	0.45	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
3	3PE	A	503	2	-	0/47/47/54	0/0/0/0
4	DXC	A	504	-	-	0/7/71/71	0/4/4/4
4	DXC	A	505	-	-	0/7/71/71	0/4/4/4
4	DXC	A	506	-	-	0/7/71/71	0/4/4/4
4	DXC	A	507	-	-	0/7/71/71	0/4/4/4
5	SO4	A	508	-	-	0/0/0/0	0/0/0/0
5	SO4	A	509	-	-	0/0/0/0	0/0/0/0
4	DXC	B	601	-	-	0/7/71/71	0/4/4/4
4	DXC	B	602	-	-	0/7/71/71	0/4/4/4
4	DXC	B	603	-	-	0/7/71/71	0/4/4/4
3	3PE	B	606	2	-	0/47/47/54	0/0/0/0
4	DXC	B	607	-	-	0/7/71/71	0/4/4/4
4	DXC	B	608	-	-	0/7/71/71	0/4/4/4
4	DXC	B	609	-	-	0/7/71/71	0/4/4/4
4	DXC	B	610	-	-	0/7/71/71	0/4/4/4
5	SO4	B	611	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	DXC	C12-C11	-4.70	1.47	1.55
4	A	507	DXC	C12-C11	-3.05	1.50	1.55
4	A	507	DXC	C12-C17	-2.97	1.50	1.55
4	B	609	DXC	C12-C11	-2.77	1.50	1.55
4	B	608	DXC	C12-C11	-2.66	1.50	1.55
4	B	608	DXC	C12-C17	-2.48	1.51	1.55
4	A	506	DXC	C12-C11	-2.46	1.51	1.55
4	B	607	DXC	C12-C13	-2.32	1.51	1.54
4	A	505	DXC	C12-C11	-2.29	1.51	1.55
4	B	602	DXC	C12-C11	-2.29	1.51	1.55
4	B	607	DXC	C4-C3	-2.28	1.51	1.55
4	B	607	DXC	C20-C12	-2.25	1.50	1.54
4	B	609	DXC	C12-C17	-2.25	1.51	1.55
4	A	504	DXC	C12-C11	-2.23	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	610	DXC	C4-C3	-2.22	1.51	1.55
4	B	601	DXC	C20-C12	-2.13	1.50	1.54
4	B	609	DXC	C12-C13	-2.12	1.51	1.54
3	A	503	3PE	O31-C3	-2.07	1.40	1.45
4	B	610	DXC	C4-C10	-2.06	1.52	1.56
4	A	507	DXC	C4-C3	-2.04	1.51	1.55
4	B	608	DXC	C12-C13	-2.01	1.51	1.54
4	A	504	DXC	C14-C13	2.13	1.57	1.53
3	A	503	3PE	O31-C31	2.29	1.40	1.33
3	B	606	3PE	O31-C31	2.80	1.41	1.33
3	A	503	3PE	O21-C21	4.09	1.46	1.34
3	B	606	3PE	O21-C21	4.61	1.47	1.34

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	DXC	C12-C11-C9	-13.77	98.73	114.70
4	A	507	DXC	C12-C11-C9	-12.78	99.87	114.70
4	B	603	DXC	C11-C9-C10	-10.72	93.89	109.09
4	A	507	DXC	C11-C9-C10	-10.21	94.61	109.09
4	B	610	DXC	C10-C14-C13	-6.57	106.13	114.38
4	A	507	DXC	C12-C17-C19	-6.26	111.81	119.44
4	B	610	DXC	C12-C11-C9	-5.52	108.29	114.70
4	B	603	DXC	C12-C17-C19	-5.09	113.24	119.44
4	B	603	DXC	C20-C12-C17	-5.02	103.29	111.20
4	A	507	DXC	C3-C2-C1	-4.44	106.31	112.88
4	B	610	DXC	C20-C12-C13	-4.31	104.78	109.09
4	B	610	DXC	C12-C17-C19	-4.21	114.30	119.44
4	B	610	DXC	C14-C13-C12	-4.17	107.01	111.22
4	B	603	DXC	C22-C21-C19	-4.12	109.69	114.79
4	B	603	DXC	C3-C2-C1	-4.02	106.93	112.88
4	B	610	DXC	C11-C9-C10	-4.01	103.40	109.09
4	B	610	DXC	C2-C3-C4	-3.93	108.44	112.66
4	B	603	DXC	C14-C10-C9	-3.91	106.12	111.12
4	B	609	DXC	O1-C13-C12	-3.89	104.62	111.12
4	B	609	DXC	C2-C3-C7	-3.85	104.23	111.67
4	A	507	DXC	C14-C10-C9	-3.80	106.27	111.12
4	A	504	DXC	C3-C2-C1	-3.73	107.36	112.88
3	B	606	3PE	O31-C31-O32	-3.50	114.33	123.51
4	B	609	DXC	C18-C4-C10	-3.49	106.58	111.20
4	A	505	DXC	C5-C6-C1	-3.47	105.79	110.41
4	B	609	DXC	C8-C9-C10	-3.44	106.00	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	608	DXC	C21-C19-C17	-3.43	103.01	110.24
4	B	607	DXC	C18-C4-C10	-3.39	106.72	111.20
4	A	507	DXC	C7-C3-C4	-3.30	106.57	112.25
3	A	503	3PE	O31-C31-O32	-3.25	114.98	123.51
4	B	603	DXC	C7-C3-C4	-3.25	106.65	112.25
4	A	505	DXC	C3-C2-C1	-3.23	108.09	112.88
4	B	601	DXC	C2-C3-C7	-3.23	105.42	111.67
4	A	507	DXC	C22-C21-C19	-3.09	110.97	114.79
4	B	601	DXC	C10-C14-C13	-3.04	110.57	114.38
4	A	506	DXC	C21-C19-C17	-3.02	103.87	110.24
4	B	610	DXC	C5-C4-C10	-3.02	106.63	111.43
4	B	609	DXC	C6-C5-C4	-3.00	107.43	112.81
4	B	607	DXC	C10-C14-C13	-2.98	110.64	114.38
3	B	606	3PE	O22-C21-C22	-2.95	112.48	123.76
4	B	603	DXC	C8-C7-C3	-2.93	105.73	111.91
4	B	607	DXC	C14-C13-C12	-2.86	108.33	111.22
4	B	608	DXC	C14-C10-C4	-2.85	110.81	113.77
4	A	507	DXC	C20-C12-C17	-2.84	106.73	111.20
4	A	505	DXC	C22-C21-C19	-2.83	111.29	114.79
4	B	610	DXC	C3-C2-C1	-2.82	108.71	112.88
4	B	603	DXC	C2-C1-C6	-2.81	106.94	110.53
4	B	603	DXC	C24-C19-C17	-2.79	108.68	112.99
4	B	608	DXC	C12-C11-C9	-2.78	111.48	114.70
4	B	609	DXC	C17-C12-C13	-2.77	115.25	117.68
4	B	608	DXC	C18-C4-C3	-2.76	105.39	110.28
4	A	505	DXC	C24-C19-C17	-2.75	108.74	112.99
3	A	503	3PE	O22-C21-C22	-2.71	113.40	123.76
4	A	506	DXC	C17-C12-C11	-2.68	97.37	100.08
4	A	507	DXC	C8-C7-C3	-2.61	106.39	111.91
3	A	503	3PE	O31-C3-C2	-2.51	101.92	108.70
4	B	607	DXC	O2-C1-C2	-2.51	104.79	109.86
4	B	608	DXC	C12-C17-C19	-2.50	116.39	119.44
4	A	507	DXC	C24-C19-C17	-2.45	109.21	112.99
4	A	504	DXC	C18-C4-C5	-2.44	104.09	108.23
4	A	507	DXC	C6-C5-C4	-2.44	108.43	112.81
4	A	504	DXC	C22-C21-C19	-2.43	111.78	114.79
3	B	606	3PE	O31-C3-C2	-2.42	102.16	108.70
4	B	601	DXC	C14-C10-C9	-2.41	108.05	111.12
4	B	607	DXC	C2-C3-C7	-2.39	107.05	111.67
4	A	507	DXC	C2-C1-C6	-2.39	107.47	110.53
4	B	610	DXC	C14-C10-C9	-2.35	108.12	111.12
4	B	610	DXC	C18-C4-C10	-2.34	108.10	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	607	DXC	C14-C10-C9	-2.33	108.15	111.12
4	A	504	DXC	C5-C6-C1	-2.32	107.32	110.41
4	B	607	DXC	C5-C4-C3	-2.32	105.21	107.76
4	A	505	DXC	C5-C4-C3	-2.30	105.23	107.76
4	A	505	DXC	C18-C4-C5	-2.28	104.36	108.23
4	B	602	DXC	C21-C19-C17	-2.27	105.46	110.24
4	B	608	DXC	C20-C12-C17	-2.26	107.65	111.20
4	B	601	DXC	C18-C4-C10	-2.21	108.28	111.20
4	A	504	DXC	C12-C17-C19	-2.20	116.76	119.44
4	A	505	DXC	C24-C19-C21	-2.15	106.84	110.33
4	B	603	DXC	C6-C5-C4	-2.14	108.96	112.81
4	B	610	DXC	C22-C21-C19	-2.13	112.16	114.79
4	A	504	DXC	C5-C4-C3	-2.13	105.42	107.76
4	B	602	DXC	C17-C12-C11	-2.12	97.94	100.08
4	B	601	DXC	C14-C13-C12	-2.12	109.08	111.22
4	B	609	DXC	C16-C17-C12	-2.11	101.55	103.59
4	B	610	DXC	C7-C8-C9	-2.09	108.60	112.07
4	B	603	DXC	C2-C3-C4	-2.09	110.42	112.66
4	B	602	DXC	C16-C17-C19	-2.06	108.83	112.12
4	B	603	DXC	C18-C4-C3	-2.06	106.64	110.28
4	B	609	DXC	C4-C10-C9	-2.06	110.10	112.41
4	B	601	DXC	C7-C8-C9	-2.01	108.74	112.07
4	A	507	DXC	C18-C4-C3	-2.01	106.73	110.28
4	B	601	DXC	C5-C4-C10	2.04	114.66	111.43
4	A	504	DXC	C11-C12-C13	2.04	109.22	107.37
3	B	606	3PE	O31-C31-C32	2.04	118.14	111.85
4	A	506	DXC	C8-C9-C10	2.08	113.17	110.47
4	A	506	DXC	C17-C12-C13	2.10	119.52	117.68
4	A	506	DXC	C12-C11-C9	2.24	117.30	114.70
4	B	610	DXC	C17-C12-C11	2.26	102.36	100.08
4	A	506	DXC	C24-C19-C21	2.29	114.04	110.33
4	B	610	DXC	C17-C12-C13	2.33	119.72	117.68
4	B	602	DXC	C10-C4-C3	2.36	112.04	108.68
4	B	608	DXC	C5-C4-C3	2.37	110.38	107.76
3	B	606	3PE	C2-O21-C21	2.38	123.81	117.91
4	A	504	DXC	O1-C13-C14	2.44	114.15	109.09
4	B	608	DXC	C10-C4-C3	2.49	112.22	108.68
4	B	603	DXC	O2-C1-C2	2.55	115.01	109.86
4	B	609	DXC	C2-C3-C4	2.56	115.40	112.66
4	A	507	DXC	C8-C9-C11	2.58	116.44	112.02
4	A	507	DXC	C5-C6-C1	2.59	113.86	110.41
4	B	601	DXC	C5-C6-C1	2.62	113.91	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	609	DXC	C10-C4-C3	2.72	112.56	108.68
4	B	607	DXC	C6-C5-C4	2.83	117.89	112.81
4	B	608	DXC	C24-C19-C21	2.84	114.94	110.33
4	A	505	DXC	C5-C4-C10	2.90	116.03	111.43
4	B	607	DXC	C5-C4-C10	2.99	116.18	111.43
4	B	603	DXC	C8-C9-C11	3.01	117.17	112.02
4	A	504	DXC	C5-C4-C10	3.10	116.35	111.43
4	B	608	DXC	C22-C21-C19	3.16	118.70	114.79
4	B	610	DXC	C10-C4-C3	3.19	113.22	108.68
4	A	507	DXC	C18-C4-C5	3.31	113.83	108.23
4	B	603	DXC	C18-C4-C5	3.33	113.87	108.23
4	B	610	DXC	C11-C12-C13	3.36	110.41	107.37
4	A	507	DXC	C14-C13-C12	3.41	114.66	111.22
4	B	603	DXC	C5-C6-C1	3.42	114.97	110.41
4	B	603	DXC	C14-C10-C4	3.64	117.55	113.77
4	A	507	DXC	C11-C12-C13	4.03	111.02	107.37
4	A	507	DXC	C14-C10-C4	4.04	117.96	113.77
4	B	609	DXC	C11-C12-C13	4.54	111.48	107.37
4	B	609	DXC	C10-C14-C13	4.75	120.35	114.38
4	B	610	DXC	C4-C10-C9	5.01	118.04	112.41
3	B	606	3PE	O21-C21-C22	5.19	122.46	111.53
4	A	507	DXC	C15-C11-C12	5.64	109.03	103.59
3	A	503	3PE	O21-C21-C22	5.99	124.15	111.53
4	B	609	DXC	C14-C13-C12	6.22	117.50	111.22
4	A	507	DXC	C8-C9-C10	6.28	118.64	110.47
4	B	603	DXC	C15-C11-C12	6.70	110.04	103.59
4	B	603	DXC	C8-C9-C10	7.12	119.73	110.47
4	B	603	DXC	C11-C12-C13	7.97	114.59	107.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	3PE	1	0
4	A	504	DXC	3	0
4	A	505	DXC	3	0
4	A	507	DXC	12	0
5	A	508	SO4	1	0
4	B	601	DXC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	DXC	2	0
4	B	603	DXC	11	0
3	B	606	3PE	1	0
4	B	607	DXC	3	0
4	B	608	DXC	2	0
4	B	609	DXC	8	0
4	B	610	DXC	8	0
5	B	611	SO4	2	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	321/393 (81%)	0.62	26 (8%) 15 12	50, 82, 135, 166	0
1	B	322/393 (81%)	0.52	15 (4%) 35 33	42, 62, 110, 134	0
All	All	643/786 (81%)	0.57	41 (6%) 23 20	42, 72, 125, 166	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ASN	7.1
1	B	72	TRP	6.6
1	B	117	GLU	5.3
1	A	72	TRP	4.5
1	A	273	LEU	4.5
1	A	62	ASP	4.4
1	B	59	LYS	4.3
1	B	62	ASP	3.9
1	A	119	GLY	3.2
1	A	278	ARG	3.2
1	A	276	TRP	3.1
1	A	57	SER	3.1
1	A	69	TRP	3.0
1	B	57	SER	3.0
1	A	246	PHE	2.9
1	B	79	ASN	2.8
1	B	118	ALA	2.8
1	B	121	ARG	2.8
1	A	296	LYS	2.8
1	A	287	TYR	2.7
1	B	61	LYS	2.7
1	A	316	PHE	2.7
1	A	144	PHE	2.7
1	A	301	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	179[A]	ASP	2.7
1	B	124	GLY	2.6
1	B	120	VAL	2.6
1	A	107	LEU	2.5
1	A	294	ILE	2.4
1	A	387	ASN	2.4
1	B	122	GLU	2.4
1	B	65	PHE	2.3
1	B	178[A]	ILE	2.3
1	A	244	VAL	2.3
1	A	298	PHE	2.2
1	A	274	GLY	2.2
1	A	243	LYS	2.1
1	A	110	TYR	2.0
1	A	142	LEU	2.0
1	A	117	GLU	2.0
1	A	308	ILE	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 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(Å <sup>2</sup> )	Q<0.9
4	DXC	B	608	28/28	0.84	0.38	14.55	44,58,69,69	28
4	DXC	B	610	28/28	0.60	0.44	7.84	67,76,81,85	28
4	DXC	B	609	28/28	0.84	0.39	5.65	49,56,72,75	28
2	ZN	B	604	1/1	0.99	0.27	4.48	60,60,60,60	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	3PE	B	606	44/51	0.97	0.25	1.86	53,68,81,93	0
4	DXC	B	607	28/28	0.95	0.23	1.65	61,69,73,76	0
3	3PE	A	503	44/51	0.95	0.26	1.49	58,69,80,98	0
4	DXC	B	601	28/28	0.95	0.21	1.19	55,71,79,80	0
2	ZN	B	605	1/1	1.00	0.23	1.08	58,58,58,58	0
2	ZN	A	502	1/1	0.99	0.22	0.92	66,66,66,66	0
2	ZN	A	501	1/1	0.98	0.20	0.71	64,64,64,64	0
4	DXC	A	505	28/28	0.96	0.19	0.05	50,54,78,86	0
4	DXC	A	504	28/28	0.95	0.19	-0.28	63,67,95,100	0
5	SO4	A	508	5/5	0.94	0.15	-1.64	52,57,63,73	5
5	SO4	B	611	5/5	0.89	0.16	-1.73	44,52,57,63	5
4	DXC	B	602	28/28	0.95	0.18	-	64,73,82,88	0
4	DXC	A	507	28/28	0.90	0.32	-	73,83,88,89	28
4	DXC	B	603	28/28	0.93	0.34	-	66,74,82,84	28
5	SO4	A	509	5/5	0.90	0.26	-	53,63,73,74	5
4	DXC	A	506	28/28	0.93	0.18	-	55,64,75,90	0

## 6.5 Other polymers

There are no such residues in this entry.