



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2017 – 11:54 PM EDT

PDB ID : 5UW6  
Title : PCY1 in Complex with Follower Peptide and Covalent Inhibitor ZPP  
Authors : Chekan, J.R.; Nair, S.K.  
Deposited on : 2017-02-20  
Resolution : 3.30 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029077

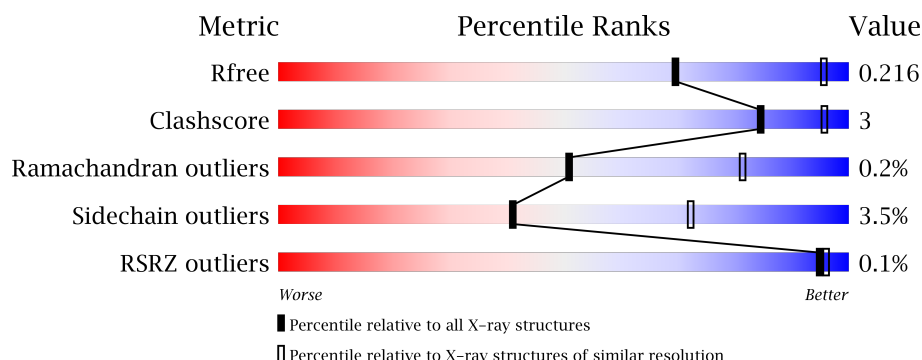
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	750	
1	B	750	
1	C	750	
1	D	750	
2	E	6	

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Mol	Chain	Length	Quality of chain
2	F	6	 100%
2	G	6	 83%17%
2	H	6	 17%83%17%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22866 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 Peptide cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	7	0
			5633	3600	957	1050	26			
1	B	706	Total	C	N	O	S	0	0	0
			5661	3617	962	1057	25			
1	C	701	Total	C	N	O	S	0	3	0
			5665	3623	966	1050	26			
1	D	697	Total	C	N	O	S	0	0	0
			5601	3582	953	1041	25			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP R4P353
A	-24	SER	-	expression tag	UNP R4P353
A	-23	TYR	-	expression tag	UNP R4P353
A	-22	TYR	-	expression tag	UNP R4P353
A	-21	HIS	-	expression tag	UNP R4P353
A	-20	HIS	-	expression tag	UNP R4P353
A	-19	HIS	-	expression tag	UNP R4P353
A	-18	HIS	-	expression tag	UNP R4P353
A	-17	HIS	-	expression tag	UNP R4P353
A	-16	HIS	-	expression tag	UNP R4P353
A	-15	LEU	-	expression tag	UNP R4P353
A	-14	GLU	-	expression tag	UNP R4P353
A	-13	SER	-	expression tag	UNP R4P353
A	-12	THR	-	expression tag	UNP R4P353
A	-11	SER	-	expression tag	UNP R4P353
A	-10	LEU	-	expression tag	UNP R4P353
A	-9	TYR	-	expression tag	UNP R4P353
A	-8	LYS	-	expression tag	UNP R4P353
A	-7	LYS	-	expression tag	UNP R4P353
A	-6	ALA	-	expression tag	UNP R4P353
A	-5	GLY	-	expression tag	UNP R4P353

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP R4P353
A	-3	GLU	-	expression tag	UNP R4P353
A	-2	PHE	-	expression tag	UNP R4P353
A	-1	ALA	-	expression tag	UNP R4P353
A	0	LEU	-	expression tag	UNP R4P353
B	-25	MET	-	initiating methionine	UNP R4P353
B	-24	SER	-	expression tag	UNP R4P353
B	-23	TYR	-	expression tag	UNP R4P353
B	-22	TYR	-	expression tag	UNP R4P353
B	-21	HIS	-	expression tag	UNP R4P353
B	-20	HIS	-	expression tag	UNP R4P353
B	-19	HIS	-	expression tag	UNP R4P353
B	-18	HIS	-	expression tag	UNP R4P353
B	-17	HIS	-	expression tag	UNP R4P353
B	-16	HIS	-	expression tag	UNP R4P353
B	-15	LEU	-	expression tag	UNP R4P353
B	-14	GLU	-	expression tag	UNP R4P353
B	-13	SER	-	expression tag	UNP R4P353
B	-12	THR	-	expression tag	UNP R4P353
B	-11	SER	-	expression tag	UNP R4P353
B	-10	LEU	-	expression tag	UNP R4P353
B	-9	TYR	-	expression tag	UNP R4P353
B	-8	LYS	-	expression tag	UNP R4P353
B	-7	LYS	-	expression tag	UNP R4P353
B	-6	ALA	-	expression tag	UNP R4P353
B	-5	GLY	-	expression tag	UNP R4P353
B	-4	SER	-	expression tag	UNP R4P353
B	-3	GLU	-	expression tag	UNP R4P353
B	-2	PHE	-	expression tag	UNP R4P353
B	-1	ALA	-	expression tag	UNP R4P353
B	0	LEU	-	expression tag	UNP R4P353
C	-25	MET	-	initiating methionine	UNP R4P353
C	-24	SER	-	expression tag	UNP R4P353
C	-23	TYR	-	expression tag	UNP R4P353
C	-22	TYR	-	expression tag	UNP R4P353
C	-21	HIS	-	expression tag	UNP R4P353
C	-20	HIS	-	expression tag	UNP R4P353
C	-19	HIS	-	expression tag	UNP R4P353
C	-18	HIS	-	expression tag	UNP R4P353
C	-17	HIS	-	expression tag	UNP R4P353
C	-16	HIS	-	expression tag	UNP R4P353
C	-15	LEU	-	expression tag	UNP R4P353

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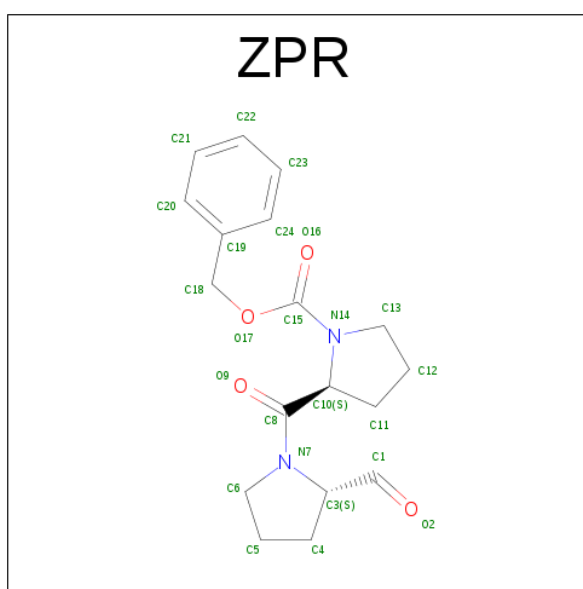
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	GLU	-	expression tag	UNP R4P353
C	-13	SER	-	expression tag	UNP R4P353
C	-12	THR	-	expression tag	UNP R4P353
C	-11	SER	-	expression tag	UNP R4P353
C	-10	LEU	-	expression tag	UNP R4P353
C	-9	TYR	-	expression tag	UNP R4P353
C	-8	LYS	-	expression tag	UNP R4P353
C	-7	LYS	-	expression tag	UNP R4P353
C	-6	ALA	-	expression tag	UNP R4P353
C	-5	GLY	-	expression tag	UNP R4P353
C	-4	SER	-	expression tag	UNP R4P353
C	-3	GLU	-	expression tag	UNP R4P353
C	-2	PHE	-	expression tag	UNP R4P353
C	-1	ALA	-	expression tag	UNP R4P353
C	0	LEU	-	expression tag	UNP R4P353
D	-25	MET	-	initiating methionine	UNP R4P353
D	-24	SER	-	expression tag	UNP R4P353
D	-23	TYR	-	expression tag	UNP R4P353
D	-22	TYR	-	expression tag	UNP R4P353
D	-21	HIS	-	expression tag	UNP R4P353
D	-20	HIS	-	expression tag	UNP R4P353
D	-19	HIS	-	expression tag	UNP R4P353
D	-18	HIS	-	expression tag	UNP R4P353
D	-17	HIS	-	expression tag	UNP R4P353
D	-16	HIS	-	expression tag	UNP R4P353
D	-15	LEU	-	expression tag	UNP R4P353
D	-14	GLU	-	expression tag	UNP R4P353
D	-13	SER	-	expression tag	UNP R4P353
D	-12	THR	-	expression tag	UNP R4P353
D	-11	SER	-	expression tag	UNP R4P353
D	-10	LEU	-	expression tag	UNP R4P353
D	-9	TYR	-	expression tag	UNP R4P353
D	-8	LYS	-	expression tag	UNP R4P353
D	-7	LYS	-	expression tag	UNP R4P353
D	-6	ALA	-	expression tag	UNP R4P353
D	-5	GLY	-	expression tag	UNP R4P353
D	-4	SER	-	expression tag	UNP R4P353
D	-3	GLU	-	expression tag	UNP R4P353
D	-2	PHE	-	expression tag	UNP R4P353
D	-1	ALA	-	expression tag	UNP R4P353
D	0	LEU	-	expression tag	UNP R4P353

- Molecule 2 is a protein called Presegetalin A1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			38	23	7	8			
2	F	6	Total	C	N	O	0	0	0
			39	23	7	9			
2	G	6	Total	C	N	O	0	0	0
			38	23	7	8			
2	H	6	Total	C	N	O	0	0	0
			39	23	7	9			

- Molecule 3 is N-BENZYLOXYCARBONYL-L-PROLYL-L-PROLINAL (three-letter code: ZPR) (formula:  $C_{18}H_{22}N_2O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	18	2	4		
3	B	1	Total	C	N	O	0	0
			24	18	2	4		
3	C	1	Total	C	N	O	0	0
			24	18	2	4		
3	D	1	Total	C	N	O	0	0
			24	18	2	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

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

- Molecule 5 is water.

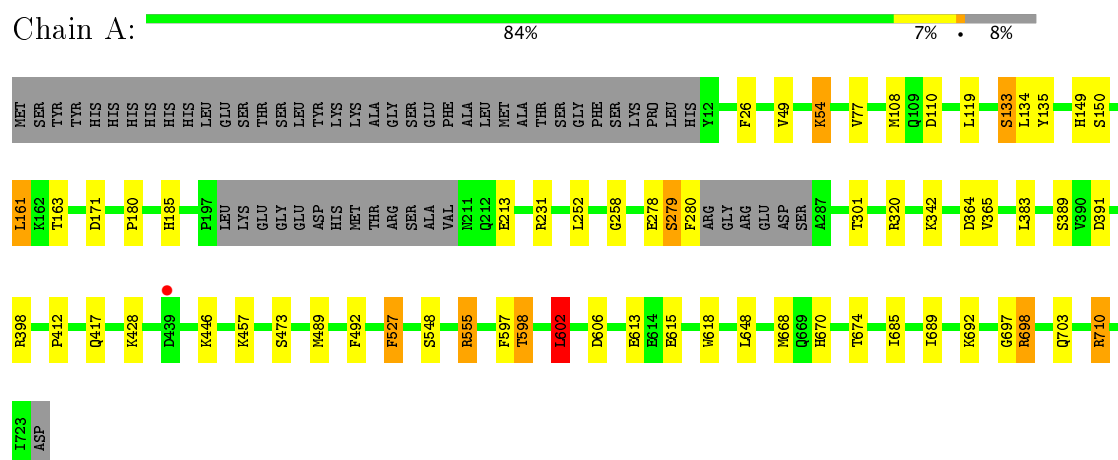
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total 13	O 13	0	0
5	B	16	Total 16	O 16	0	0
5	C	8	Total 8	O 8	0	0
5	D	15	Total 15	O 15	0	0



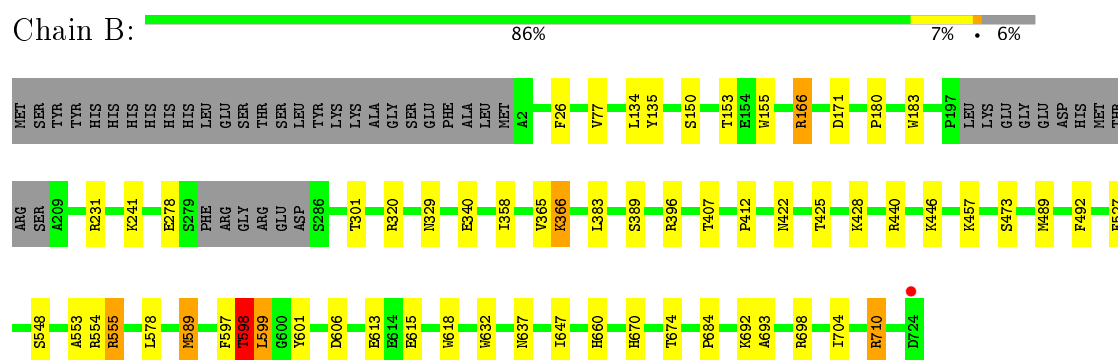
### 3 Residue-property plots

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

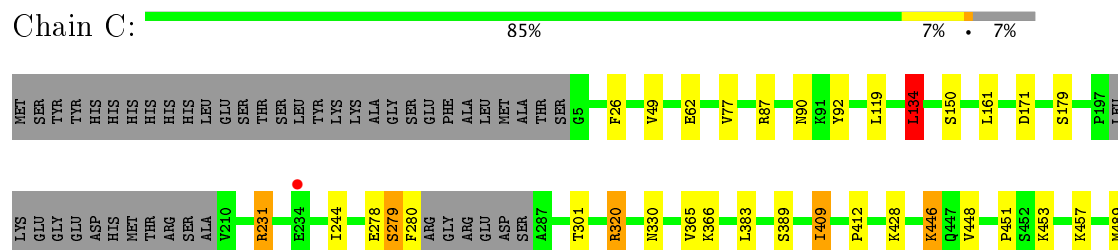
- Molecule 1: Peptide cyclase 1

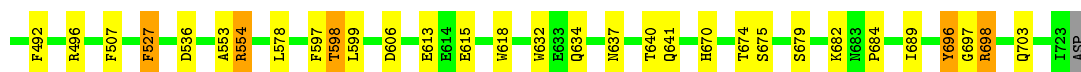


- Molecule 1: Peptide cyclase 1



- Molecule 1: Peptide cyclase 1





- Molecule 1: Peptide cyclase 1

Chain D: 86% 7% 7%



- Molecule 2: Presegetalin A1

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: Presegetalin A1

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: Presegetalin A1

Chain G: 83% 17%



- Molecule 2: Presegetalin A1

Chain H: 17% 83% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.51Å 85.46Å 138.12Å 87.60° 78.17° 89.38°	Depositor
Resolution (Å)	45.20 – 3.30 45.23 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.20-3.30) 97.7 (45.23-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.172 , 0.220 0.173 , 0.216	Depositor DCC
$R_{free}$ test set	2089 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-k,h-l 0.015 for -h,k,-l 0.009 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: CA, ZPR

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	0.56	0/5777	0.74	4/7821 (0.1%)
1	B	0.55	0/5807	0.75	8/7866 (0.1%)
1	C	0.57	0/5812	0.76	8/7869 (0.1%)
1	D	0.56	1/5746 (0.0%)	0.73	4/7781 (0.1%)
2	E	0.55	0/38	0.49	0/52
2	F	0.56	0/39	0.56	0/52
2	G	0.60	0/38	0.62	0/52
2	H	0.64	0/39	0.50	0/52
All	All	0.56	1/23296 (0.0%)	0.74	24/31545 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	639	GLU	CG-CD	5.44	1.60	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	LEU	CA-CB-CG	10.58	139.63	115.30
1	B	704	ILE	CA-CB-CG1	7.57	125.39	111.00
1	A	161	LEU	CA-CB-CG	7.09	131.60	115.30
1	C	134	LEU	CB-CG-CD2	6.40	121.88	111.00
1	B	599	LEU	CA-CB-CG	6.39	129.99	115.30
1	B	598	THR	CB-CA-C	-6.24	94.75	111.60
1	C	554[A]	ARG	CA-CB-CG	6.14	126.92	113.40
1	C	554[B]	ARG	CA-CB-CG	6.14	126.92	113.40
1	A	602	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	166	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	589	MET	N-CA-C	-5.88	95.12	111.00
1	C	320	ARG	N-CA-C	-5.56	95.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	589	MET	N-CA-C	-5.52	96.11	111.00
1	B	555	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	D	496	ARG	CG-CD-NE	5.42	123.18	111.80
1	D	398	ARG	CB-CA-C	-5.32	99.77	110.40
1	D	320	ARG	N-CA-C	-5.26	96.78	111.00
1	A	320	ARG	N-CA-C	-5.20	96.96	111.00
1	C	134	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	B	710	ARG	CG-CD-NE	-5.10	101.08	111.80
1	A	710	ARG	CG-CD-NE	-5.06	101.18	111.80
1	C	161	LEU	CB-CA-C	-5.05	100.61	110.20
1	C	231	ARG	N-CA-C	5.04	124.60	111.00
1	B	710	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	5633	0	5472	34	0
1	B	5661	0	5502	28	0
1	C	5665	0	5512	39	0
1	D	5601	0	5449	29	0
2	E	38	0	36	0	0
2	F	39	0	36	0	0
2	G	38	0	36	1	0
2	H	39	0	36	1	0
3	A	24	0	21	0	0
3	B	24	0	21	0	0
3	C	24	0	21	0	0
3	D	24	0	21	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	13	0	0	0	0
5	B	16	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	8	0	0	2	0
5	D	15	0	0	2	0
All	All	22866	0	22163	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (122) 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:C:682:LYS:HG2	5:C:901:HOH:O	1.81	0.79
1:D:587:GLY:C	1:D:589:MET:HE2	2.10	0.72
1:C:446:LYS:HE3	1:C:448:VAL:CG1	2.23	0.67
1:A:342:LYS:HD2	1:C:366:LYS:HE3	1.77	0.67
1:A:698:ARG:HD3	1:A:703:GLN:OE1	1.97	0.65
1:C:446:LYS:HE3	1:C:448:VAL:HG13	1.81	0.62
1:C:446:LYS:CE	1:C:448:VAL:CG1	2.77	0.62
1:A:668:MET:HB3	1:A:685[B]:ILE:HD13	1.83	0.61
1:B:320:ARG:O	1:B:340:GLU:HG3	2.02	0.60
1:D:473:SER:O	1:D:555:ARG:NH2	2.35	0.59
1:B:647:ILE:HG23	5:B:907:HOH:O	2.03	0.58
1:D:448:VAL:HG22	1:D:449:PHE:N	2.17	0.58
1:D:224:SER:OG	5:D:901:HOH:O	1.96	0.58
1:A:258:GLY:HA2	1:A:602:LEU:HB2	1.84	0.58
1:C:279:SER:O	1:C:280:PHE:CG	2.57	0.57
1:A:668:MET:CB	1:A:685[B]:ILE:HD13	2.34	0.57
1:B:134:LEU:HD12	1:B:135:TYR:N	2.21	0.55
1:A:110:ASP:HB3	1:D:271:THR:HB	1.87	0.55
1:A:364:ASP:OD2	1:C:457:LYS:HE2	2.06	0.55
1:D:587:GLY:HA3	1:D:589:MET:CE	2.37	0.54
1:D:134:LEU:HD12	1:D:135:TYR:N	2.23	0.54
1:D:134:LEU:HD13	1:D:180:PRO:HA	1.89	0.54
1:A:134:LEU:HD12	1:A:135:TYR:N	2.23	0.53
1:C:696:TYR:CD2	1:C:697:GLY:N	2.76	0.53
1:A:134:LEU:HD13	1:A:180:PRO:HA	1.90	0.53
1:C:679:SER:O	5:C:901:HOH:O	2.19	0.52
1:B:134:LEU:HD13	1:B:180:PRO:HA	1.91	0.52
1:B:396:ARG:NH2	5:B:901:HOH:O	2.32	0.51
1:D:589:MET:O	1:D:660:HIS:ND1	2.44	0.51
1:B:553:ALA:O	1:B:578:LEU:O	2.29	0.50
1:C:446:LYS:CE	1:C:448:VAL:HG12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:GLY:HA3	1:D:589:MET:HE3	1.92	0.50
1:D:553:ALA:O	1:D:578:LEU:O	2.30	0.50
1:B:407:THR:CG2	1:B:492:PHE:H	2.25	0.49
1:A:108:MET:CE	1:A:163:THR:HB	2.42	0.49
1:A:670:HIS:HA	1:A:674:THR:OG1	2.13	0.49
1:C:670:HIS:HA	1:C:674:THR:OG1	2.12	0.49
1:D:670:HIS:HA	1:D:674:THR:OG1	2.12	0.49
1:B:598:THR:OG1	1:B:598:THR:O	2.10	0.49
1:A:698:ARG:CD	1:A:703:GLN:OE1	2.61	0.48
1:C:446:LYS:HE2	1:C:448:VAL:CG1	2.43	0.48
1:C:553:ALA:O	1:C:578:LEU:O	2.31	0.48
1:C:598:THR:HB	1:C:599:LEU:HD12	1.95	0.48
1:C:698:ARG:H	1:C:698:ARG:HD2	1.78	0.48
1:C:703:GLN:HG3	2:G:32:VAL:HG21	1.96	0.48
1:A:108:MET:SD	1:A:119:LEU:HD13	2.54	0.48
1:B:613:GLU:HB3	1:D:617:LYS:NZ	2.29	0.47
1:C:615:GLU:HG2	1:C:618:TRP:CH2	2.49	0.47
1:D:615:GLU:HG2	1:D:618:TRP:CH2	2.50	0.47
1:D:26:PHE:CD1	1:D:613:GLU:HB2	2.50	0.47
1:B:366:LYS:HE3	5:B:912:HOH:O	2.15	0.47
1:B:670:HIS:HA	1:B:674:THR:OG1	2.14	0.47
1:B:183:TRP:HB3	5:B:906:HOH:O	2.14	0.47
1:C:26:PHE:CD1	1:C:613:GLU:HB2	2.50	0.47
1:B:589:MET:O	1:B:660:HIS:ND1	2.47	0.46
1:C:446:LYS:HE3	1:C:448:VAL:HG12	1.96	0.46
1:B:599:LEU:HA	1:B:601:TYR:CE1	2.51	0.46
1:A:279:SER:O	1:A:280:PHE:CG	2.69	0.46
1:A:473:SER:O	1:A:555:ARG:NH1	2.49	0.46
1:B:473:SER:O	1:B:555:ARG:NH1	2.49	0.46
1:A:26:PHE:CD1	1:A:613:GLU:HB2	2.52	0.45
1:C:87[A]:ARG:HE	1:C:90:ASN:HA	1.81	0.45
1:B:597:PHE:O	1:B:598:THR:C	2.54	0.45
1:A:597:PHE:O	1:A:598:THR:C	2.55	0.45
1:C:412:PRO:HA	1:C:492:PHE:CG	2.51	0.45
1:A:278:GLU:O	1:A:279:SER:C	2.55	0.45
1:C:670:HIS:CD2	1:C:675:SER:HB3	2.52	0.45
1:D:138:SER:HB2	5:D:903:HOH:O	2.17	0.45
1:B:26:PHE:CD1	1:B:613:GLU:HB2	2.52	0.44
1:A:279:SER:O	1:A:280:PHE:CB	2.66	0.44
1:A:615:GLU:HG2	1:A:618:TRP:CH2	2.53	0.44
1:B:615:GLU:HG2	1:B:618:TRP:CH2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:SER:HB2	1:B:489:MET:HB3	2.00	0.44
1:A:412:PRO:HA	1:A:492:PHE:CG	2.53	0.44
1:B:422:ASN:OD1	1:C:330:ASN:ND2	2.51	0.44
1:D:597:PHE:O	1:D:598:THR:C	2.57	0.43
1:A:668:MET:HB2	1:A:685[B]:ILE:CD1	2.49	0.43
1:C:597:PHE:O	1:C:598:THR:C	2.56	0.43
1:D:161:LEU:HD11	1:D:168:TYR:CE1	2.54	0.43
1:D:648:LEU:N	1:D:648:LEU:HD12	2.32	0.43
1:D:527:PHE:C	1:D:527:PHE:CD1	2.92	0.43
1:C:134:LEU:HD12	1:C:179:SER:O	2.19	0.42
1:D:412:PRO:HA	1:D:492:PHE:CG	2.53	0.42
1:A:389:SER:HB2	1:A:489:MET:HB3	2.01	0.42
1:C:49:VAL:HG13	1:C:689:ILE:HD13	2.01	0.42
1:D:448:VAL:CG2	1:D:449:PHE:N	2.82	0.42
1:C:632:TRP:HA	1:C:637:ASN:O	2.19	0.42
1:A:527:PHE:CD1	1:A:527:PHE:C	2.91	0.42
1:B:440:ARG:HG3	1:B:440:ARG:HH11	1.84	0.42
1:C:87[A]:ARG:HD3	1:C:92:TYR:CZ	2.54	0.42
1:A:685[B]:ILE:O	1:A:685[B]:ILE:HG13	2.12	0.42
1:C:409:ILE:HD12	1:C:496:ARG:NH1	2.34	0.42
1:A:457:LYS:HB3	1:C:451:PRO:HD3	2.01	0.42
1:C:698:ARG:HD3	1:C:703:GLN:OE1	2.20	0.42
1:A:133:SER:HB2	1:A:149:HIS:HE1	1.85	0.41
1:A:213:GLU:HG2	1:A:231:ARG:HG2	2.02	0.41
1:B:153:THR:HG23	1:B:155:TRP:H	1.85	0.41
1:B:412:PRO:HA	1:B:492:PHE:CG	2.54	0.41
1:A:108:MET:HE1	1:A:163:THR:HB	2.01	0.41
1:B:632:TRP:HA	1:B:637:ASN:O	2.20	0.41
1:A:49:VAL:HG13	1:A:689:ILE:HD13	2.02	0.41
1:C:527:PHE:CD1	1:C:527:PHE:C	2.93	0.41
1:D:49:VAL:HG13	1:D:689:ILE:HD13	2.03	0.41
1:D:587:GLY:C	1:D:589:MET:CE	2.86	0.41
1:A:391:ASP:C	1:A:391:ASP:OD1	2.59	0.41
1:B:329:ASN:O	1:D:331:PRO:HD2	2.20	0.41
1:B:693:ALA:HB1	1:B:698:ARG:HD2	2.02	0.41
1:D:632:TRP:HA	1:D:637:ASN:O	2.20	0.41
1:C:640:THR:CG2	1:C:641:GLN:N	2.84	0.41
1:A:54:LYS:CD	1:A:54:LYS:C	2.89	0.41
1:B:366:LYS:HB3	5:B:912:HOH:O	2.20	0.41
1:C:278:GLU:O	1:C:279:SER:C	2.55	0.41
1:C:134:LEU:CD1	1:C:179:SER:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:SER:OG	2:H:32:VAL:OXT	2.31	0.41
1:A:252:LEU:HD12	1:A:252:LEU:N	2.36	0.41
1:C:279:SER:O	1:C:280:PHE:CB	2.69	0.40
1:C:389:SER:HB2	1:C:489:MET:HB3	2.03	0.40
1:B:613:GLU:HB3	1:D:617:LYS:HZ2	1.86	0.40
1:C:453:LYS:HE2	1:C:536:ASP:OD1	2.22	0.40
1:C:496:ARG:HD3	1:C:507:PHE:CD2	2.57	0.40
1:A:648:LEU:HD12	1:A:648:LEU:N	2.36	0.40
1:D:473:SER:O	1:D:555:ARG:CZ	2.69	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	694/750 (92%)	658 (95%)	34 (5%)	2 (0%)	44	76
1	B	700/750 (93%)	663 (95%)	36 (5%)	1 (0%)	55	85
1	C	698/750 (93%)	662 (95%)	34 (5%)	2 (0%)	44	76
1	D	691/750 (92%)	654 (95%)	36 (5%)	1 (0%)	55	85
2	E	4/6 (67%)	4 (100%)	0	0	100	100
2	F	4/6 (67%)	4 (100%)	0	0	100	100
2	G	4/6 (67%)	4 (100%)	0	0	100	100
2	H	4/6 (67%)	4 (100%)	0	0	100	100
All	All	2799/3024 (93%)	2653 (95%)	140 (5%)	6 (0%)	51	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	THR

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Mol	Chain	Res	Type
1	A	697	GLY
1	B	598	THR
1	C	598	THR
1	C	696	TYR
1	D	598	THR

### 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	610/652 (94%)	587 (96%)	23 (4%)	38	70
1	B	613/652 (94%)	590 (96%)	23 (4%)	38	70
1	C	613/652 (94%)	590 (96%)	23 (4%)	38	70
1	D	606/652 (93%)	589 (97%)	17 (3%)	49	76
2	E	4/4 (100%)	4 (100%)	0	100	100
2	F	4/4 (100%)	4 (100%)	0	100	100
2	G	4/4 (100%)	4 (100%)	0	100	100
2	H	4/4 (100%)	4 (100%)	0	100	100
All	All	2458/2624 (94%)	2372 (96%)	86 (4%)	41	72

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	77	VAL
1	A	133	SER
1	A	150	SER
1	A	161	LEU
1	A	171	ASP
1	A	185	HIS
1	A	279	SER
1	A	301	THR
1	A	365	VAL

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Mol	Chain	Res	Type
1	A	383	LEU
1	A	398	ARG
1	A	417	GLN
1	A	428	LYS
1	A	446	LYS
1	A	527	PHE
1	A	548	SER
1	A	555	ARG
1	A	602	LEU
1	A	606	ASP
1	A	692	LYS
1	A	698	ARG
1	A	710	ARG
1	B	77	VAL
1	B	150	SER
1	B	166	ARG
1	B	171	ASP
1	B	231	ARG
1	B	241	LYS
1	B	278	GLU
1	B	301	THR
1	B	358	ILE
1	B	365	VAL
1	B	366	LYS
1	B	383	LEU
1	B	425	THR
1	B	428	LYS
1	B	446	LYS
1	B	457	LYS
1	B	527	PHE
1	B	548	SER
1	B	554	ARG
1	B	606	ASP
1	B	684	PRO
1	B	692	LYS
1	B	710	ARG
1	C	62	GLU
1	C	77	VAL
1	C	119	LEU
1	C	134	LEU
1	C	150	SER
1	C	171	ASP

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Mol	Chain	Res	Type
1	C	231	ARG
1	C	244	ILE
1	C	279	SER
1	C	301	THR
1	C	320	ARG
1	C	365	VAL
1	C	383	LEU
1	C	409	ILE
1	C	428	LYS
1	C	446	LYS
1	C	527	PHE
1	C	554[A]	ARG
1	C	554[B]	ARG
1	C	606	ASP
1	C	634	GLN
1	C	684	PRO
1	C	698	ARG
1	D	7	SER
1	D	77	VAL
1	D	119	LEU
1	D	133	SER
1	D	161	LEU
1	D	171	ASP
1	D	185	HIS
1	D	231	ARG
1	D	290	MET
1	D	301	THR
1	D	365	VAL
1	D	425	THR
1	D	428	LYS
1	D	527	PHE
1	D	554	ARG
1	D	606	ASP
1	D	698	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	109	GLN
1	A	149	HIS
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	670	HIS
2	E	27	ASN
1	B	107	GLN
1	B	670	HIS
2	F	27	ASN
1	D	670	HIS

### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ZPR	A	801	1	25,26,26	1.23	1 (4%)	32,35,35	2.35	3 (9%)
3	ZPR	B	801	1	25,26,26	1.51	1 (4%)	32,35,35	1.69	6 (18%)
3	ZPR	C	801	1	25,26,26	1.31	1 (4%)	32,35,35	2.58	4 (12%)
3	ZPR	D	801	1	25,26,26	1.42	1 (4%)	32,35,35	2.34	6 (18%)

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	ZPR	A	801	1	-	0/17/39/39	0/3/3/3
3	ZPR	B	801	1	-	0/17/39/39	0/3/3/3
3	ZPR	C	801	1	-	1/17/39/39	0/3/3/3
3	ZPR	D	801	1	-	1/17/39/39	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ZPR	O17-C15	5.09	1.44	1.34
3	C	801	ZPR	O17-C15	5.88	1.45	1.34
3	B	801	ZPR	O17-C15	6.31	1.46	1.34
3	D	801	ZPR	O17-C15	6.37	1.46	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ZPR	O17-C15-O16	-6.05	114.33	124.83
3	C	801	ZPR	O17-C15-O16	-5.98	114.45	124.83
3	C	801	ZPR	C4-C3-C1	-5.91	104.58	112.70
3	D	801	ZPR	O17-C15-O16	-4.68	116.71	124.83
3	B	801	ZPR	O17-C15-O16	-3.04	119.55	124.83
3	D	801	ZPR	C4-C3-C1	-2.46	109.32	112.70
3	D	801	ZPR	O2-C1-C3	-2.26	117.40	124.50
3	B	801	ZPR	O2-C1-C3	-2.16	117.73	124.50
3	B	801	ZPR	C12-C13-N14	2.11	106.50	103.22
3	D	801	ZPR	C4-C3-N7	2.16	104.29	101.98
3	B	801	ZPR	O17-C18-C19	2.20	114.88	109.41
3	D	801	ZPR	C13-N14-C15	2.27	128.60	122.94
3	C	801	ZPR	C4-C3-N7	2.76	104.93	101.98
3	A	801	ZPR	C4-C3-N7	3.00	105.18	101.98
3	B	801	ZPR	C18-O17-C15	3.08	124.45	115.65
3	B	801	ZPR	O17-C15-N14	5.94	116.92	111.08
3	C	801	ZPR	O17-C15-N14	10.28	121.18	111.08
3	D	801	ZPR	O17-C15-N14	10.28	121.18	111.08
3	A	801	ZPR	O17-C15-N14	10.28	121.19	111.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	801	ZPR	C18-O17-C15-N14
3	D	801	ZPR	C18-O17-C15-N14

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	693/750 (92%)	-0.35	1 (0%) 95 96	15, 32, 59, 97	0
1	B	706/750 (94%)	-0.36	1 (0%) 95 96	17, 30, 58, 92	0
1	C	701/750 (93%)	-0.41	1 (0%) 95 96	10, 28, 56, 97	0
1	D	697/750 (92%)	-0.39	0 100 100	15, 30, 57, 91	0
2	E	6/6 (100%)	-0.49	0 100 100	33, 41, 52, 56	0
2	F	6/6 (100%)	-0.01	0 100 100	27, 36, 53, 55	0
2	G	6/6 (100%)	0.14	0 100 100	30, 36, 56, 57	0
2	H	6/6 (100%)	0.16	1 (16%) 2 2	28, 32, 51, 62	0
All	All	2821/3024 (93%)	-0.38	4 (0%) 95 96	10, 30, 58, 97	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	27	ASN	2.6
1	A	439	ASP	2.4
1	B	724	ASP	2.2
1	C	234	GLU	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(Å <sup>2</sup> )	Q<0.9
3	ZPR	A	801	24/24	0.94	0.25	1.26	41,54,58,62	0
3	ZPR	B	801	24/24	0.94	0.21	0.81	26,31,56,58	0
3	ZPR	D	801	24/24	0.95	0.20	0.57	33,40,52,53	0
3	ZPR	C	801	24/24	0.94	0.20	0.16	31,37,48,48	0
4	CA	A	802	1/1	0.97	0.12	-2.25	41,41,41,41	0
4	CA	B	803	1/1	0.92	0.06	-2.37	30,30,30,30	0
4	CA	B	802	1/1	0.85	0.09	-	37,37,37,37	0
4	CA	C	802	1/1	0.96	0.05	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.