



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:25 am BST

PDB ID : 5UW3  
Title : PCY1 in Complex with Follower Peptide  
Authors : Chekan, J.R.; Nair, S.K.  
Deposited on : 2017-02-20  
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

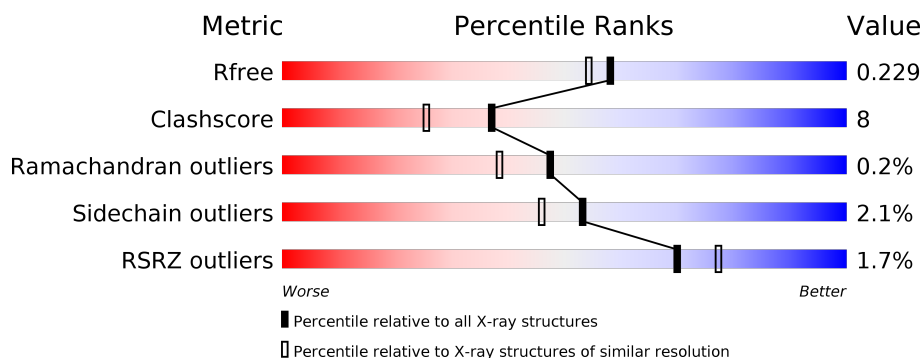
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	750	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
1	B	750	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	C	750	<div> <div></div> <div> <div></div> <div>81%</div> <div>11%</div> <div>6%</div> </div> </div>
1	D	750	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>
2	E	19	<div> <div></div> <div> <div>26%</div> <div>5%</div> <div>68%</div> </div> </div>
2	F	19	<div> <div></div> <div> <div>26%</div> <div>5%</div> <div>68%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	19	 21% 11% 68%
2	H	19	 32% 68%

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
3	CAC	C	801	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24731 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	0	0
			5573	3564	946	1038	25			
1	B	707	Total	C	N	O	S	0	0	0
			5669	3622	963	1058	26			
1	C	702	Total	C	N	O	S	0	0	0
			5646	3612	961	1048	25			
1	D	698	Total	C	N	O	S	0	0	0
			5608	3586	954	1043	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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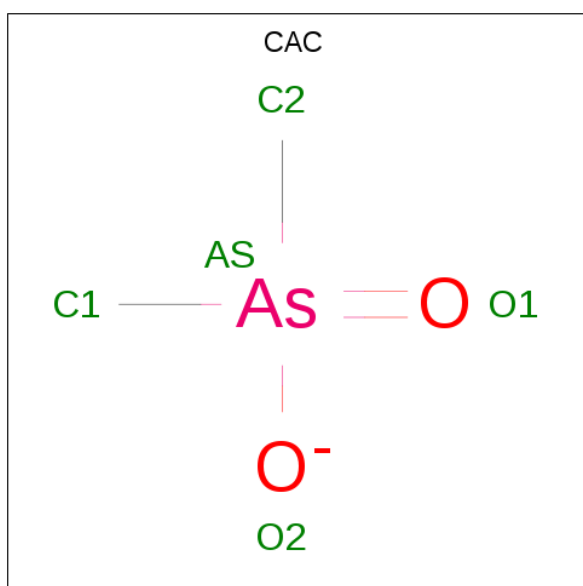
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	GLU	-	expression tag	UNP R4P353
C	-13	SER	-	expression tag	UNP R4P353
C	-12	THR	-	expression tag	UNP R4P353
C	-11	SER	-	expression tag	UNP R4P353
C	-10	LEU	-	expression tag	UNP R4P353
C	-9	TYR	-	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 CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	C	1	Total	As	C	O	0	0
			5	1	2	2		
3	D	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	451	Total	O	0	0
			451	451		
4	E	6	Total	O	0	0
			6	6		

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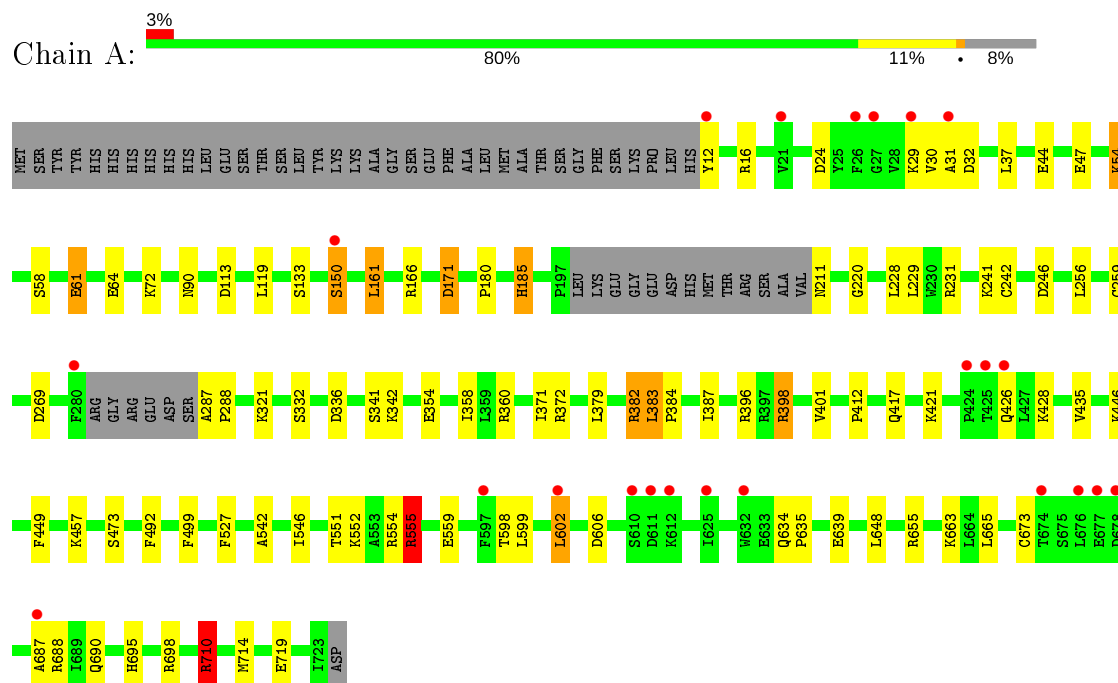
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	491	Total 491	O 491	0	0
4	F	5	Total 5	O 5	0	0
4	C	563	Total 563	O 563	0	0
4	G	5	Total 5	O 5	0	0
4	D	535	Total 535	O 535	0	0
4	H	5	Total 5	O 5	0	0



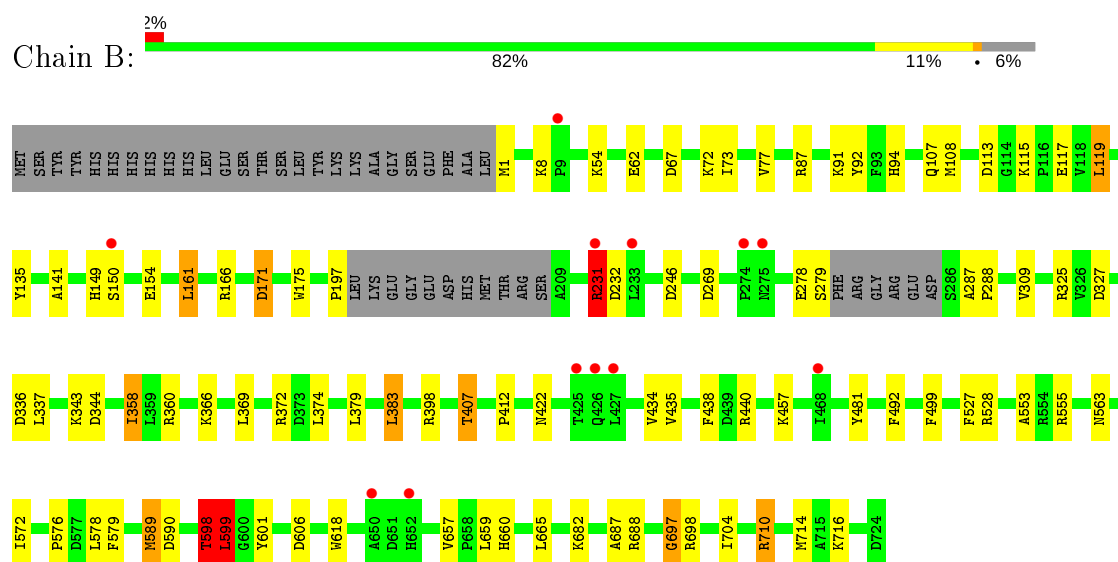
### 3 Residue-property plots [i](#)

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







GLY	
VAL	
PRO	
VAL	
TRP	
ALA	
PHE	
GLN	
ALA	
LYS	
ASP	
VAL	
GLU	
N1027	
V1032	

● Molecule 2: Presegetalin A1



GLY	
VAL	
PRO	
VAL	
TRP	
ALA	
PHE	
GLN	
ALA	
LYS	
ASP	
VAL	
GLU	
N1027	
V1032	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.50Å 85.59Å 137.72Å 87.41° 78.28° 89.33°	Depositor
Resolution (Å)	44.90 – 1.96 44.91 – 1.96	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.90-1.96) 95.8 (44.91-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.189 , 0.224 0.195 , 0.229	Depositor DCC
$R_{free}$ test set	9945 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.086 for h,-k,h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC

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	0.83	0/5717	0.86	13/7743 (0.2%)
1	B	0.83	2/5815 (0.0%)	0.89	18/7876 (0.2%)
1	C	0.87	3/5793 (0.1%)	0.90	22/7845 (0.3%)
1	D	0.87	4/5753 (0.1%)	0.92	13/7791 (0.2%)
2	E	0.99	0/38	0.72	0/52
2	F	0.98	0/39	0.68	0/52
2	G	0.99	0/38	0.74	0/52
2	H	0.89	0/39	0.75	0/52
All	All	0.85	9/23232 (0.0%)	0.89	66/31463 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	608	GLY	N-CA	10.86	1.62	1.46
1	C	608	GLY	N-CA	10.67	1.62	1.46
1	B	618	TRP	CB-CG	-7.13	1.37	1.50
1	D	496	ARG	CD-NE	-6.31	1.35	1.46
1	C	136	SER	CB-OG	-5.75	1.34	1.42
1	D	590	ASP	N-CA	5.72	1.57	1.46
1	C	481	TYR	CZ-OH	5.43	1.47	1.37
1	B	407	THR	CB-CG2	-5.35	1.34	1.52
1	D	614	GLU	CD-OE1	5.24	1.31	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	496	ARG	NE-CZ-NH2	-14.50	113.05	120.30
1	D	607	TYR	C-N-CA	-12.52	96.01	122.30
1	C	607	TYR	C-N-CA	-12.06	96.97	122.30
1	D	496	ARG	NE-CZ-NH1	11.56	126.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	161	LEU	CA-CB-CG	7.31	132.11	115.30
1	D	590	ASP	N-CA-CB	7.22	123.59	110.60
1	D	607	TYR	O-C-N	-7.11	111.11	123.20
1	C	607	TYR	O-C-N	-7.11	111.12	123.20
1	A	336	ASP	CB-CG-OD1	7.09	124.69	118.30
1	B	161	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	161	LEU	CB-CG-CD1	-6.68	99.64	111.00
1	D	336	ASP	CB-CG-OD1	6.64	124.27	118.30
1	B	710	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	360	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	589	MET	O-C-N	-6.50	112.30	122.70
1	B	598	THR	CB-CA-C	-6.49	94.08	111.60
1	D	496	ARG	CD-NE-CZ	6.46	132.65	123.60
1	C	396	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	360	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	134	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	599	LEU	CA-CB-CG	6.28	129.75	115.30
1	B	336	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	590	ASP	N-CA-CB	6.09	121.56	110.60
1	A	269	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	171	ASP	CB-CG-OD1	5.98	123.69	118.30
1	B	360	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	113	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	589	MET	O-C-N	-5.79	113.43	122.70
1	C	290	MET	CG-SD-CE	5.78	109.45	100.20
1	C	231	ARG	N-CA-C	5.78	126.60	111.00
1	A	698	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	528	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	710	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	D	269	ASP	CB-CG-OD1	5.55	123.30	118.30
1	D	246	ASP	CB-CG-OD2	5.51	123.25	118.30
1	B	232	ASP	N-CA-C	5.47	125.78	111.00
1	A	246	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	555	ARG	CG-CD-NE	-5.46	100.34	111.80
1	A	710	ARG	CD-NE-CZ	5.42	131.19	123.60
1	C	336	ASP	CB-CG-OD1	5.37	123.14	118.30
1	C	161	LEU	CA-CB-CG	5.33	127.55	115.30
1	C	87	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	16	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	688	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	229	LEU	CA-CB-CG	5.30	127.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	607	TYR	CA-C-N	5.29	126.78	116.20
1	A	171	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	589	MET	N-CA-C	-5.28	96.75	111.00
1	C	269	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	232	ASP	N-CA-C	5.27	125.23	111.00
1	C	320	ARG	CD-NE-CZ	5.21	130.90	123.60
1	C	593	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	398	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	688	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	231	ARG	N-CA-C	5.16	124.92	111.00
1	C	396	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	B	269	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	327	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	C	327	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	688	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	67	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	528	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	246	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	589	MET	CG-SD-CE	5.04	108.26	100.20

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	5573	0	5417	113	1
1	B	5669	0	5515	80	0
1	C	5646	0	5494	70	0
1	D	5608	0	5457	87	1
2	E	38	0	36	1	0
2	F	39	0	36	1	0
2	G	38	0	36	2	0
2	H	39	0	36	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	3	0
3	C	5	0	0	4	0
3	D	5	0	0	1	0
4	A	451	0	0	58	0
4	B	491	0	0	43	0
4	C	563	0	0	27	0
4	D	535	0	0	46	0
4	E	6	0	0	1	0
4	F	5	0	0	1	0
4	G	5	0	0	1	0
4	H	5	0	0	0	0
All	All	24731	0	22027	350	1

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 8.

All (350) 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:321:LYS:HE3	4:A:905:HOH:O	1.31	1.30
1:B:714:MET:SD	4:B:1318:HOH:O	1.99	1.18
1:D:714:MET:SD	4:D:1365:HOH:O	1.95	1.18
1:C:422:ASN:CG	4:C:902:HOH:O	1.81	1.16
1:D:588:VAL:C	1:D:589:MET:HE2	1.69	1.12
1:B:325:ARG:HB2	4:B:1294:HOH:O	1.46	1.12
1:B:161:LEU:HB3	4:B:1326:HOH:O	1.46	1.12
4:B:991:HOH:O	1:C:375:GLU:HG3	1.51	1.11
1:D:297:ASP:HB3	4:D:1326:HOH:O	1.51	1.10
1:B:161:LEU:CB	4:B:1326:HOH:O	2.00	1.09
1:A:321:LYS:CE	4:A:905:HOH:O	1.89	1.07
1:A:714:MET:SD	4:A:1291:HOH:O	2.09	1.06
1:A:599:LEU:HD21	1:A:655:ARG:HA	1.36	1.05
1:D:161:LEU:HB3	4:D:1334:HOH:O	1.58	1.03
1:A:663:LYS:HG2	4:A:1227:HOH:O	1.63	0.99
1:B:576:PRO:HA	4:B:1282:HOH:O	1.63	0.99
1:A:673:CYS:SG	4:A:929:HOH:O	2.05	0.98
1:B:337:LEU:HB2	4:B:1294:HOH:O	1.66	0.96
1:A:663:LYS:CG	4:A:1227:HOH:O	2.14	0.96
1:B:231:ARG:O	4:B:901:HOH:O	1.85	0.92
1:D:135:TYR:C	4:D:908:HOH:O	2.06	0.91
1:A:599:LEU:O	1:A:602:LEU:HD23	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:HD21	4:B:1312:HOH:O	1.70	0.91
1:B:438:PHE:CE2	1:B:440:ARG:HG2	2.04	0.91
1:C:246:ASP:OD1	4:C:901:HOH:O	1.89	0.90
1:C:723:ILE:C	4:C:1063:HOH:O	2.09	0.90
1:C:320:ARG:NH1	1:C:341:SER:O	2.05	0.88
1:B:481:TYR:OH	3:B:801:CAC:C2	2.23	0.87
1:D:211:ASN:N	4:D:902:HOH:O	2.05	0.87
1:A:259:CYS:SG	1:A:602:LEU:HD12	2.14	0.86
1:D:572:ILE:HA	4:D:1240:HOH:O	1.74	0.85
1:C:434:VAL:HG23	4:C:1128:HOH:O	1.76	0.85
1:D:588:VAL:C	1:D:589:MET:CE	2.45	0.85
2:F:1027:ASN:N	4:F:1101:HOH:O	2.09	0.84
1:B:72:LYS:HD3	4:B:1303:HOH:O	1.77	0.84
1:B:589:MET:O	1:B:660:HIS:ND1	2.10	0.83
1:D:496:ARG:HD2	1:D:507:PHE:CG	2.12	0.83
1:A:599:LEU:H	1:A:599:LEU:HD23	1.44	0.83
1:A:499:PHE:HE1	1:A:714:MET:HE3	1.43	0.83
4:A:1160:HOH:O	1:D:249:LYS:HD2	1.77	0.83
1:D:230:TRP:CD1	4:D:919:HOH:O	2.31	0.82
1:C:422:ASN:ND2	4:C:902:HOH:O	2.00	0.82
1:D:185:HIS:HE1	4:D:1345:HOH:O	1.62	0.82
1:D:589:MET:O	1:D:660:HIS:ND1	2.11	0.81
1:A:499:PHE:CE1	1:A:714:MET:HE3	2.16	0.80
1:B:553:ALA:O	1:B:578:LEU:O	2.00	0.79
1:C:287:ALA:N	4:C:904:HOH:O	2.14	0.79
1:C:563:ASN:H	3:C:801:CAC:C1	1.96	0.79
1:C:142:LYS:HG2	1:C:164:GLU:OE2	1.83	0.78
1:A:398:ARG:HG2	4:A:925:HOH:O	1.82	0.78
1:B:91:LYS:HG3	4:B:1109:HOH:O	1.82	0.77
1:D:211:ASN:N	4:D:904:HOH:O	2.17	0.77
1:C:409:ILE:HD12	1:C:496:ARG:NH1	2.00	0.76
3:D:801:CAC:O2	4:D:901:HOH:O	2.04	0.76
1:A:648:LEU:HD21	4:A:1322:HOH:O	1.86	0.75
1:D:576:PRO:HA	4:D:1240:HOH:O	1.86	0.75
1:C:149:HIS:HD2	4:C:917:HOH:O	1.67	0.75
1:A:499:PHE:CE1	1:A:714:MET:CE	2.70	0.74
1:A:16:ARG:HG2	4:A:1079:HOH:O	1.87	0.73
1:D:287:ALA:N	4:D:906:HOH:O	2.21	0.73
1:D:499:PHE:CE1	1:D:714:MET:CE	2.71	0.73
1:D:297:ASP:CB	4:D:1326:HOH:O	2.18	0.73
1:D:588:VAL:O	1:D:589:MET:CE	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:THR:OG1	1:B:598:THR:O	2.00	0.73
1:D:589:MET:HE2	1:D:589:MET:N	2.05	0.72
1:B:499:PHE:CE1	1:B:714:MET:CE	2.72	0.72
1:A:710:ARG:HB3	4:A:1322:HOH:O	1.89	0.72
1:B:374:LEU:HD22	4:B:1014:HOH:O	1.89	0.71
1:D:579:PHE:HD2	4:D:1240:HOH:O	1.72	0.71
1:D:499:PHE:HE1	1:D:714:MET:HE3	1.56	0.71
1:A:228:LEU:HD11	1:A:231:ARG:CG	2.21	0.71
1:B:438:PHE:CE2	1:B:440:ARG:CG	2.75	0.70
1:D:553:ALA:O	1:D:578:LEU:O	2.08	0.70
1:A:90:ASN:HB3	4:D:1328:HOH:O	1.90	0.70
1:D:588:VAL:O	1:D:589:MET:HE1	1.90	0.70
1:C:481:TYR:OH	3:C:801:CAC:C1	2.40	0.69
1:D:473:SER:O	1:D:555:ARG:NH2	2.25	0.69
1:A:180:PRO:HG2	4:A:1284:HOH:O	1.92	0.69
1:B:343:LYS:HG2	1:B:344:ASP:OD1	1.93	0.69
1:C:290:MET:HB3	4:C:1407:HOH:O	1.93	0.69
1:B:572:ILE:HA	4:B:1282:HOH:O	1.93	0.68
1:A:710:ARG:CB	4:A:1322:HOH:O	2.42	0.68
1:D:499:PHE:CE1	1:D:714:MET:HE3	2.29	0.68
1:C:210:VAL:N	4:C:908:HOH:O	2.26	0.68
1:A:180:PRO:HD2	4:A:1284:HOH:O	1.93	0.68
1:A:37:LEU:HB2	4:A:1227:HOH:O	1.95	0.67
1:B:499:PHE:CE1	1:B:714:MET:HE1	2.29	0.67
1:B:407:THR:CG2	1:B:492:PHE:H	2.07	0.67
1:A:30:VAL:O	4:A:903:HOH:O	2.12	0.67
1:A:719:GLU:OE1	4:A:904:HOH:O	2.13	0.67
1:B:117:GLU:HB3	1:B:166:ARG:HH21	1.59	0.67
1:A:256:LEU:HD13	4:A:1012:HOH:O	1.94	0.67
1:A:387:ILE:HG22	4:A:976:HOH:O	1.95	0.66
1:B:499:PHE:HE1	1:B:714:MET:HE3	1.58	0.66
1:A:58:SER:O	1:A:61:GLU:OE1	2.14	0.66
1:D:136:SER:N	4:D:908:HOH:O	2.26	0.66
1:D:191:PHE:CE1	1:D:229:LEU:HD21	2.30	0.66
1:D:499:PHE:CE1	1:D:714:MET:HE1	2.31	0.66
1:D:496:ARG:HD2	1:D:507:PHE:CD1	2.30	0.66
4:B:1130:HOH:O	1:C:421:LYS:HE2	1.96	0.66
1:A:342:LYS:HB3	4:A:1308:HOH:O	1.96	0.65
1:A:47:GLU:HG3	4:A:1210:HOH:O	1.94	0.65
1:A:599:LEU:HB2	1:A:602:LEU:CD2	2.27	0.65
1:A:599:LEU:CD2	1:A:655:ARG:HA	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HA	1:A:47:GLU:HG2	1.79	0.65
1:D:191:PHE:HE1	1:D:229:LEU:HD21	1.62	0.64
1:D:343:LYS:HG2	1:D:344:ASP:OD1	1.96	0.64
1:B:113:ASP:OD1	4:B:903:HOH:O	2.15	0.64
1:B:154:GLU:O	4:B:904:HOH:O	2.15	0.64
1:D:618:TRP:CZ2	4:D:949:HOH:O	2.50	0.64
1:C:136:SER:HB2	4:C:1359:HOH:O	1.97	0.64
1:A:64:GLU:OE2	4:A:906:HOH:O	2.15	0.64
1:A:354:GLU:HG2	4:A:1268:HOH:O	1.98	0.63
1:A:710:ARG:NE	4:A:901:HOH:O	1.96	0.63
1:B:117:GLU:HG2	4:B:1274:HOH:O	1.99	0.63
1:D:159:LYS:HE3	4:D:1054:HOH:O	1.98	0.62
1:A:332:SER:HB3	4:A:1279:HOH:O	2.00	0.62
1:A:90:ASN:HB3	4:D:932:HOH:O	1.98	0.62
1:D:161:LEU:HD23	4:D:1334:HOH:O	2.00	0.61
1:B:107:GLN:HB3	4:B:912:HOH:O	2.00	0.61
1:B:555:ARG:HD3	4:B:1201:HOH:O	1.99	0.61
1:B:499:PHE:CD1	1:B:714:MET:HE1	2.35	0.61
1:B:563:ASN:H	3:B:801:CAC:C2	2.13	0.61
1:D:496:ARG:HD2	1:D:507:PHE:CD2	2.35	0.61
1:B:499:PHE:CE1	1:B:714:MET:HE3	2.33	0.61
1:D:423:ASP:OD2	1:D:426:GLN:NE2	2.34	0.61
1:D:698:ARG:HD2	4:D:1062:HOH:O	2.00	0.61
1:B:161:LEU:HD13	4:B:1326:HOH:O	2.00	0.60
1:A:358:ILE:HG12	1:A:371:ILE:CD1	2.31	0.60
1:B:698:ARG:HG2	4:B:1356:HOH:O	2.02	0.60
1:D:499:PHE:CD1	1:D:714:MET:HE1	2.37	0.60
1:A:228:LEU:HD11	1:A:231:ARG:HG2	1.83	0.59
1:D:588:VAL:N	1:D:589:MET:HE2	2.17	0.59
1:B:457:LYS:HG3	4:B:914:HOH:O	2.02	0.59
1:B:87:ARG:CZ	4:B:916:HOH:O	2.50	0.59
1:A:180:PRO:CG	4:A:1284:HOH:O	2.50	0.59
1:B:94:HIS:HD2	4:B:1029:HOH:O	1.85	0.59
1:D:90:ASN:HB2	4:D:1351:HOH:O	2.02	0.58
1:C:440:ARG:NH2	4:C:903:HOH:O	2.11	0.58
1:A:559:GLU:HG2	4:A:911:HOH:O	2.03	0.58
1:A:663:LYS:HG3	4:A:1227:HOH:O	1.95	0.58
1:B:499:PHE:HE1	1:B:714:MET:CE	2.15	0.58
1:C:451:PRO:HA	4:C:1328:HOH:O	2.02	0.58
1:C:546:ILE:HD13	1:C:551:THR:HG23	1.85	0.58
1:D:698:ARG:HG2	4:D:1406:HOH:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ASP:HB2	4:C:986:HOH:O	2.04	0.57
1:C:446:LYS:HE3	1:C:447:GLN:O	2.04	0.57
1:B:161:LEU:HB2	4:B:1326:HOH:O	1.88	0.57
1:A:710:ARG:CD	4:A:1322:HOH:O	2.53	0.56
1:A:166:ARG:NH1	4:A:922:HOH:O	2.39	0.56
1:A:449:PHE:HB2	4:C:1328:HOH:O	2.04	0.56
1:A:473:SER:O	1:A:555:ARG:NH1	2.38	0.56
1:A:32:ASP:N	4:A:903:HOH:O	2.38	0.56
1:A:384:PRO:HG2	1:C:342:LYS:HB2	1.86	0.56
1:A:546:ILE:HD13	1:A:551:THR:HG23	1.88	0.55
1:C:134:LEU:CD1	1:C:179:SER:O	2.55	0.55
1:C:553:ALA:O	1:C:578:LEU:O	2.24	0.55
1:D:249:LYS:NZ	4:D:912:HOH:O	2.36	0.55
1:A:382:ARG:HH22	1:C:382:ARG:NH2	2.04	0.55
1:B:598:THR:O	1:B:599:LEU:HG	2.06	0.55
1:C:438:PHE:HD1	4:C:1382:HOH:O	1.88	0.55
1:D:650:ALA:HB2	1:D:698:ARG:NH2	2.21	0.55
1:A:321:LYS:NZ	4:A:905:HOH:O	2.14	0.55
1:A:599:LEU:HD21	1:A:655:ARG:CA	2.23	0.55
1:C:546:ILE:CD1	1:C:551:THR:HG23	2.37	0.55
1:A:412:PRO:HG3	1:A:435:VAL:HG23	1.90	0.54
1:B:87:ARG:NE	4:B:916:HOH:O	2.40	0.54
1:C:703:GLN:HG3	2:G:1032:VAL:HG21	1.90	0.54
1:D:618:TRP:CE2	4:D:949:HOH:O	2.59	0.54
1:B:161:LEU:CD1	4:B:1326:HOH:O	2.51	0.54
1:D:520:GLU:HG3	1:D:524:LYS:HE2	1.89	0.54
1:C:191:PHE:CE2	1:C:244:ILE:HD11	2.42	0.54
1:C:87:ARG:HG3	1:C:88:ARG:N	2.22	0.54
1:B:309:VAL:HG13	4:B:1290:HOH:O	2.08	0.54
1:D:614:GLU:C	4:D:949:HOH:O	2.46	0.54
1:C:446:LYS:HD3	1:C:448:VAL:HG13	1.90	0.54
1:D:218:PHE:HE2	1:D:227:ILE:HD11	1.72	0.54
1:B:422:ASN:OD1	1:C:330:ASN:ND2	2.31	0.53
1:B:412:PRO:HG3	1:B:435:VAL:HG23	1.89	0.53
1:B:62:GLU:CG	1:B:716:LYS:NZ	2.70	0.53
1:B:682:LYS:HE2	4:B:930:HOH:O	2.09	0.53
1:A:398:ARG:NE	4:A:925:HOH:O	2.42	0.53
1:B:438:PHE:CZ	1:B:440:ARG:HG2	2.41	0.53
1:C:47:GLU:HG3	4:C:1277:HOH:O	2.07	0.53
1:D:166:ARG:HB2	4:D:1353:HOH:O	2.08	0.53
1:B:73:ILE:CG2	1:B:704:ILE:HD12	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:OD2	1:A:29:LYS:NZ	2.35	0.52
1:A:710:ARG:HD2	4:A:1322:HOH:O	2.10	0.52
1:D:412:PRO:HG3	1:D:435:VAL:HG23	1.91	0.52
1:A:401:VAL:HG13	1:A:401:VAL:O	2.09	0.52
1:D:316:LYS:HE3	4:D:1326:HOH:O	2.09	0.52
1:D:614:GLU:HG2	1:D:615:GLU:N	2.24	0.52
1:C:356:GLN:NE2	1:C:380:GLN:OE1	2.42	0.52
1:C:412:PRO:HG3	1:C:435:VAL:HG23	1.92	0.52
1:C:375:GLU:OE2	1:C:375:GLU:HA	2.09	0.52
1:D:230:TRP:NE1	4:D:919:HOH:O	2.41	0.52
1:A:54:LYS:HD2	1:A:54:LYS:O	2.10	0.52
1:A:673:CYS:N	4:A:929:HOH:O	2.42	0.52
1:A:710:ARG:NH2	4:A:901:HOH:O	2.42	0.52
1:C:197:PRO:HD2	4:C:1394:HOH:O	2.09	0.52
1:D:4:SER:O	4:D:905:HOH:O	2.18	0.52
1:A:12:TYR:HB3	4:A:1107:HOH:O	2.09	0.51
1:A:546:ILE:CD1	1:A:551:THR:HG23	2.40	0.51
1:A:90:ASN:CB	4:D:1328:HOH:O	2.54	0.51
1:B:92:TYR:OH	4:B:905:HOH:O	2.19	0.51
1:C:412:PRO:HA	1:C:492:PHE:CG	2.44	0.51
1:A:499:PHE:CE1	1:A:714:MET:HE1	2.42	0.51
1:A:599:LEU:N	1:A:599:LEU:HD23	2.18	0.51
1:C:546:ILE:HD12	1:C:552:LYS:HA	1.92	0.51
1:D:697:GLY:HA3	4:D:1077:HOH:O	2.11	0.51
1:A:119:LEU:CD1	1:A:161:LEU:HD11	2.41	0.50
1:B:279:SER:C	4:B:1041:HOH:O	2.49	0.50
1:B:87:ARG:NH1	4:B:925:HOH:O	2.45	0.50
1:A:211:ASN:N	4:A:937:HOH:O	2.45	0.50
1:A:31:ALA:C	4:A:903:HOH:O	2.50	0.50
1:B:366:LYS:HG2	4:B:1003:HOH:O	2.10	0.50
1:A:119:LEU:HD11	1:A:161:LEU:HD11	1.94	0.50
1:A:341:SER:CB	4:A:907:HOH:O	2.58	0.50
1:C:136:SER:CB	4:C:1359:HOH:O	2.58	0.50
1:A:457:LYS:HE2	1:C:449:PHE:HB2	1.93	0.50
1:C:129:ARG:NH1	4:C:921:HOH:O	2.45	0.50
1:D:166:ARG:HD3	4:D:1353:HOH:O	2.11	0.49
1:A:228:LEU:HD11	1:A:231:ARG:HG3	1.94	0.49
1:A:499:PHE:CD1	1:A:714:MET:HE1	2.47	0.49
1:D:499:PHE:HE1	1:D:714:MET:CE	2.15	0.49
1:A:37:LEU:HD12	4:A:1227:HOH:O	2.11	0.49
1:C:191:PHE:HE2	1:C:244:ILE:HD11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:HIS:HD2	4:D:962:HOH:O	1.96	0.49
1:D:588:VAL:CA	1:D:589:MET:HE2	2.40	0.49
1:B:54:LYS:HG3	4:B:1321:HOH:O	2.11	0.49
1:A:180:PRO:CD	4:A:1284:HOH:O	2.55	0.49
1:B:698:ARG:N	4:B:929:HOH:O	2.46	0.49
1:B:710:ARG:NH2	4:B:902:HOH:O	2.45	0.49
1:B:149:HIS:HE1	4:B:904:HOH:O	1.96	0.48
1:B:358:ILE:HD11	1:B:369:LEU:HB3	1.96	0.48
1:A:166:ARG:HD3	4:A:922:HOH:O	2.14	0.48
1:D:161:LEU:CB	4:D:1334:HOH:O	2.32	0.48
1:C:8:LYS:HE3	1:C:62:GLU:CG	2.44	0.48
1:A:417:GLN:OE1	1:A:428:LYS:NZ	2.46	0.48
1:A:690:GLN:OE1	4:A:908:HOH:O	2.20	0.48
1:C:134:LEU:HD12	1:C:179:SER:O	2.14	0.48
1:C:409:ILE:HD12	1:C:496:ARG:HH11	1.77	0.47
1:A:412:PRO:HA	1:A:492:PHE:CG	2.48	0.47
1:A:473:SER:C	4:A:1096:HOH:O	2.52	0.47
1:D:412:PRO:HA	1:D:492:PHE:CG	2.50	0.47
1:D:259:CYS:HB2	4:D:1148:HOH:O	2.14	0.47
1:A:401:VAL:HG11	4:A:1000:HOH:O	2.14	0.47
1:B:412:PRO:HA	1:B:492:PHE:CG	2.50	0.47
1:B:62:GLU:HG2	1:B:716:LYS:NZ	2.30	0.47
1:D:554:ARG:CZ	1:D:554:ARG:CB	2.93	0.47
1:B:287:ALA:HB1	1:B:288:PRO:HD2	1.96	0.46
1:A:287:ALA:HB1	1:A:288:PRO:HD2	1.97	0.46
1:C:287:ALA:HB1	1:C:288:PRO:HD2	1.96	0.46
1:D:698:ARG:N	4:D:922:HOH:O	2.43	0.46
1:A:372:ARG:HG2	1:A:379:LEU:HA	1.97	0.46
1:C:446:LYS:CD	1:C:448:VAL:HG13	2.45	0.46
1:D:195:TYR:OH	4:D:903:HOH:O	2.07	0.46
1:A:499:PHE:HE1	1:A:714:MET:CE	2.12	0.46
1:A:546:ILE:HD12	1:A:552:LYS:HA	1.97	0.46
1:C:383:LEU:HD23	4:C:955:HOH:O	2.15	0.46
1:C:423:ASP:OD2	1:C:426:GLN:HG3	2.15	0.45
1:B:327:ASP:HB2	4:B:1290:HOH:O	2.16	0.45
1:D:698:ARG:HB2	4:D:1062:HOH:O	2.15	0.45
1:D:161:LEU:HD11	1:D:168:TYR:CZ	2.51	0.45
1:A:259:CYS:SG	1:A:602:LEU:CD1	2.99	0.45
1:C:211:ASN:HB3	4:C:993:HOH:O	2.16	0.45
1:C:562:SER:CB	3:C:801:CAC:C1	2.95	0.45
1:C:562:SER:HB3	3:C:801:CAC:C1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LEU:CD1	1:D:168:TYR:CD2	3.00	0.45
1:D:614:GLU:CG	4:D:949:HOH:O	2.65	0.45
1:A:648:LEU:CD2	4:A:1322:HOH:O	2.52	0.45
2:G:1027:ASN:N	4:G:1101:HOH:O	2.49	0.45
1:A:220:GLY:HA2	4:A:1102:HOH:O	2.17	0.45
1:B:579:PHE:HD2	4:B:1282:HOH:O	2.00	0.45
1:C:372:ARG:HG2	1:C:379:LEU:HA	1.98	0.45
1:D:491:THR:O	1:D:496:ARG:NH2	2.50	0.44
1:B:135:TYR:O	1:B:135:TYR:CD2	2.70	0.44
1:B:73:ILE:HG21	1:B:704:ILE:HD12	1.99	0.44
1:A:665:LEU:HD22	1:A:687:ALA:HB2	1.98	0.44
1:A:401:VAL:CG1	1:A:401:VAL:O	2.65	0.44
1:D:287:ALA:HB1	1:D:288:PRO:HD2	2.00	0.44
1:D:135:TYR:HB2	4:D:908:HOH:O	2.17	0.44
1:D:161:LEU:HD11	1:D:168:TYR:CE2	2.53	0.44
1:A:446:LYS:CE	4:A:1048:HOH:O	2.65	0.44
1:A:449:PHE:HB3	1:A:457:LYS:HG3	2.00	0.44
1:A:44:GLU:CA	1:A:47:GLU:HG2	2.46	0.44
1:C:255:ILE:HB	1:C:264:LYS:HB2	2.00	0.44
1:D:604:THR:O	1:D:607:TYR:O	2.36	0.43
1:C:665:LEU:HD22	1:C:687:ALA:HB2	1.99	0.43
1:C:8:LYS:HE3	1:C:62:GLU:CD	2.39	0.43
1:A:54:LYS:HD2	1:A:54:LYS:C	2.39	0.43
1:D:372:ARG:HG2	1:D:379:LEU:HA	2.00	0.43
1:A:655:ARG:HD2	1:A:695:HIS:CD2	2.54	0.43
1:B:665:LEU:HD22	1:B:687:ALA:HB2	2.01	0.43
1:D:655:ARG:HD2	1:D:695:HIS:CD2	2.54	0.43
1:B:108:MET:HE2	1:B:119:LEU:HD13	1.99	0.43
1:B:62:GLU:HG3	1:B:716:LYS:NZ	2.33	0.43
1:D:554:ARG:HB3	1:D:554:ARG:NH1	2.34	0.43
1:A:166:ARG:CD	4:A:922:HOH:O	2.66	0.42
1:B:117:GLU:HB3	1:B:166:ARG:NH2	2.31	0.42
1:A:673:CYS:CB	4:A:929:HOH:O	2.53	0.42
1:B:115:LYS:HD3	4:B:986:HOH:O	2.18	0.42
1:D:614:GLU:HG2	1:D:615:GLU:HG3	2.01	0.42
1:B:141:ALA:HB1	4:B:1109:HOH:O	2.18	0.42
1:B:481:TYR:CZ	3:B:801:CAC:C2	3.01	0.42
1:B:278:GLU:O	1:B:279:SER:C	2.58	0.42
1:C:47:GLU:HB2	4:C:1075:HOH:O	2.19	0.42
1:C:87:ARG:HE	1:C:90:ASN:HA	1.84	0.42
1:D:453:LYS:HG3	4:D:1037:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:ARG:CB	4:D:1062:HOH:O	2.67	0.42
1:A:341:SER:HB2	4:A:907:HOH:O	2.19	0.42
1:C:281:ARG:O	4:C:906:HOH:O	2.21	0.42
1:C:639:GLU:OE1	4:C:905:HOH:O	2.21	0.42
1:D:72:LYS:HD2	4:D:1301:HOH:O	2.20	0.42
1:A:37:LEU:CD1	4:A:1227:HOH:O	2.66	0.42
1:D:448:VAL:HG22	1:D:449:PHE:N	2.34	0.42
1:D:166:ARG:CG	4:D:1353:HOH:O	2.67	0.42
1:D:599:LEU:C	1:D:599:LEU:HD12	2.40	0.42
1:C:527:PHE:C	1:C:527:PHE:CD1	2.93	0.42
1:B:372:ARG:HG2	1:B:379:LEU:HA	2.01	0.41
4:A:1160:HOH:O	1:D:307:GLY:HA2	2.19	0.41
1:C:546:ILE:HD12	1:C:552:LYS:CA	2.50	0.41
1:A:44:GLU:O	1:A:47:GLU:HG2	2.19	0.41
1:A:634:GLN:HA	1:A:635:PRO:HD3	1.97	0.41
1:B:161:LEU:CD2	1:B:166:ARG:O	2.68	0.41
1:A:396:ARG:NE	4:A:915:HOH:O	2.34	0.41
1:B:710:ARG:NE	4:B:902:HOH:O	1.99	0.41
1:C:613:GLU:OE2	4:C:907:HOH:O	2.22	0.41
1:C:655:ARG:HD2	1:C:695:HIS:CD2	2.55	0.41
2:E:1027:ASN:N	4:E:1101:HOH:O	2.53	0.41
1:A:546:ILE:HD12	1:A:552:LYS:CA	2.50	0.41
1:B:175:TRP:CD1	1:B:197:PRO:HA	2.56	0.41
1:A:599:LEU:N	1:A:599:LEU:CD2	2.84	0.41
1:C:129:ARG:NH2	1:C:151:GLY:O	2.54	0.41
1:C:542:ALA:O	1:C:546:ILE:HG12	2.21	0.41
1:A:44:GLU:O	1:A:47:GLU:CG	2.69	0.41
1:B:657:VAL:HG23	1:B:659:LEU:HG	2.03	0.41
1:A:383:LEU:HA	4:A:1203:HOH:O	2.21	0.41
1:B:697:GLY:HA3	4:B:1111:HOH:O	2.21	0.41
1:B:599:LEU:HA	1:B:601:TYR:CE2	2.56	0.41
1:D:161:LEU:CG	4:D:1334:HOH:O	2.65	0.41
1:A:150:SER:N	4:A:923:HOH:O	2.39	0.40
1:A:542:ALA:O	1:A:546:ILE:HG12	2.21	0.40
1:C:553:ALA:HB3	4:C:950:HOH:O	2.19	0.40
1:D:161:LEU:CD1	1:D:168:TYR:CE2	3.04	0.40
1:C:134:LEU:HD23	4:C:1359:HOH:O	2.21	0.40
1:A:241:LYS:HG3	1:A:242:CYS:N	2.36	0.40
1:A:58:SER:HA	1:A:61:GLU:OE1	2.21	0.40
1:D:255:ILE:HB	1:D:264:LYS:HB2	2.03	0.40
1:A:72:LYS:HD2	4:A:974:HOH:O	2.21	0.40



All (1) 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)
1:A:554:ARG:NH2	1:D:638:GLU:OE1[1_456]	2.12	0.08

## 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	687/750 (92%)	666 (97%)	20 (3%)	1 (0%)	51	43
1	B	701/750 (94%)	676 (96%)	23 (3%)	2 (0%)	41	30
1	C	696/750 (93%)	673 (97%)	21 (3%)	2 (0%)	41	30
1	D	692/750 (92%)	671 (97%)	20 (3%)	1 (0%)	51	43
2	E	4/19 (21%)	4 (100%)	0	0	100	100
2	F	4/19 (21%)	4 (100%)	0	0	100	100
2	G	4/19 (21%)	4 (100%)	0	0	100	100
2	H	4/19 (21%)	4 (100%)	0	0	100	100
All	All	2792/3076 (91%)	2702 (97%)	84 (3%)	6 (0%)	47	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	598	THR
1	C	279	SER
1	C	598	THR
1	A	598	THR
1	D	598	THR
1	B	697	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/652 (92%)	586 (97%)	17 (3%)	43	33
1	B	614/652 (94%)	601 (98%)	13 (2%)	53	46
1	C	611/652 (94%)	601 (98%)	10 (2%)	62	58
1	D	607/652 (93%)	596 (98%)	11 (2%)	59	53
2	E	4/14 (29%)	4 (100%)	0	100	100
2	F	4/14 (29%)	4 (100%)	0	100	100
2	G	4/14 (29%)	4 (100%)	0	100	100
2	H	4/14 (29%)	4 (100%)	0	100	100
All	All	2451/2664 (92%)	2400 (98%)	51 (2%)	53	46

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	61	GLU
1	A	133	SER
1	A	150	SER
1	A	171	ASP
1	A	185	HIS
1	A	229	LEU
1	A	383	LEU
1	A	398	ARG
1	A	421	LYS
1	A	426	GLN
1	A	527	PHE
1	A	555	ARG
1	A	602	LEU
1	A	606	ASP
1	A	639	GLU
1	A	710	ARG
1	B	1	MET
1	B	8	LYS

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Mol	Chain	Res	Type
1	B	77	VAL
1	B	119	LEU
1	B	150	SER
1	B	171	ASP
1	B	231	ARG
1	B	358	ILE
1	B	383	LEU
1	B	434	VAL
1	B	527	PHE
1	B	599	LEU
1	B	606	ASP
1	C	62	GLU
1	C	171	ASP
1	C	231	ARG
1	C	234	GLU
1	C	383	LEU
1	C	396	ARG
1	C	446	LYS
1	C	527	PHE
1	C	555	ARG
1	C	606	ASP
1	D	61	GLU
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	428	LYS
1	D	527	PHE
1	D	554	ARG
1	D	606	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	185	HIS
1	A	595	HIS
1	B	94	HIS
1	B	149	HIS
1	B	381	HIS

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Mol	Chain	Res	Type
1	C	149	HIS
1	C	185	HIS
1	C	652	HIS
1	C	670	HIS
1	D	185	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	CAC	D	801	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	B	801	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	C	801	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	A	801	-	0,4,4	0.00	-	0,6,6	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	CAC	1	0
3	B	801	CAC	3	0
3	C	801	CAC	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.19	23 (3%) 46 56	8, 20, 41, 58	0
1	B	707/750 (94%)	-0.05	12 (1%) 70 77	8, 17, 39, 59	0
1	C	702/750 (93%)	-0.14	3 (0%) 92 95	7, 15, 34, 63	0
1	D	698/750 (93%)	-0.12	10 (1%) 75 82	7, 16, 34, 74	0
2	E	6/19 (31%)	-0.23	0 100 100	13, 14, 16, 18	0
2	F	6/19 (31%)	-0.36	0 100 100	12, 14, 17, 19	0
2	G	6/19 (31%)	-0.10	0 100 100	15, 16, 20, 20	0
2	H	6/19 (31%)	-0.33	0 100 100	13, 14, 18, 19	0
All	All	2824/3076 (91%)	-0.03	48 (1%) 70 77	7, 17, 37, 74	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	THR	7.9
1	D	425	THR	4.3
1	A	150	SER	3.8
1	A	625	ILE	3.7
1	A	677	GLU	3.7
1	D	274	PRO	3.6
1	A	611	ASP	3.4
1	A	597	PHE	3.4
1	A	676	LEU	3.2
1	A	425	THR	3.1
1	B	233	LEU	3.1
1	D	426	GLN	3.0
1	A	29	LYS	2.9
1	A	280	PHE	2.8
1	A	26	PHE	2.7
1	A	674	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	610	SER	2.7
1	B	275	ASN	2.6
1	A	31	ALA	2.5
1	A	612	LYS	2.5
1	D	150	SER	2.5
1	A	602	LEU	2.4
1	C	9	PRO	2.4
1	B	426	GLN	2.4
1	A	21	VAL	2.4
1	A	426	GLN	2.3
1	B	468	ILE	2.3
1	C	8	LYS	2.3
1	A	687	ALA	2.3
1	D	677	GLU	2.3
1	B	9	PRO	2.3
1	B	652	HIS	2.2
1	A	632	TRP	2.2
1	B	427	LEU	2.2
1	A	678	ASP	2.2
1	A	424	PRO	2.2
1	D	697	GLY	2.2
1	D	275	ASN	2.2
1	B	150	SER	2.1
1	C	150	SER	2.1
1	B	274	PRO	2.1
1	D	287	ALA	2.1
1	D	166	ARG	2.1
1	B	425	THR	2.0
1	A	12	TYR	2.0
1	B	650	ALA	2.0
1	B	231	ARG	2.0
1	A	27	GLY	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CAC	B	801	5/5	0.99	0.10	17,21,25,25	0
3	CAC	C	801	5/5	0.99	0.08	14,17,18,20	0
3	CAC	A	801	5/5	0.99	0.06	24,25,28,28	0
3	CAC	D	801	5/5	1.00	0.05	15,16,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.