



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:36 pm BST

PDB ID : 4WL2  
Title : Structure of penicillin V acylase from *Pectobacterium atrosepticum*  
Authors : Ramasamy, S.; Avinash, V.S.; Pundle, A.V.; Suresh, C.G.  
Deposited on : 2014-10-06  
Resolution : 2.50 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  
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

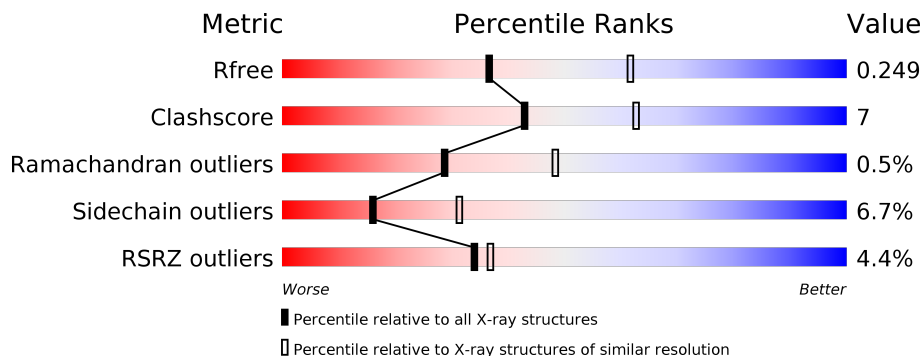
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



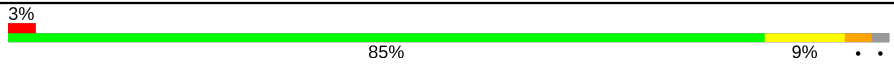

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	355	
1	B	355	
1	C	355	
1	D	355	
1	E	355	
1	F	355	

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Mol	Chain	Length	Quality of chain
1	G	355	
1	H	355	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 21734 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 Putative exported choloylglycine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2711	1730	462	513	6	0	0	0
1	B	347	2711	1730	462	513	6	0	0	0
1	C	347	2711	1730	462	513	6	0	0	0
1	D	347	2711	1730	462	513	6	0	0	0
1	E	347	2711	1730	462	513	6	0	0	0
1	F	347	2711	1730	462	513	6	0	0	0
1	G	347	2711	1730	462	513	6	0	0	0
1	H	347	2711	1730	462	513	6	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	348	LEU	-	expression tag	UNP Q6D291
A	349	GLU	-	expression tag	UNP Q6D291
A	350	HIS	-	expression tag	UNP Q6D291
A	351	HIS	-	expression tag	UNP Q6D291
A	352	HIS	-	expression tag	UNP Q6D291
A	353	HIS	-	expression tag	UNP Q6D291
A	354	HIS	-	expression tag	UNP Q6D291
A	355	HIS	-	expression tag	UNP Q6D291
B	348	LEU	-	expression tag	UNP Q6D291
B	349	GLU	-	expression tag	UNP Q6D291
B	350	HIS	-	expression tag	UNP Q6D291
B	351	HIS	-	expression tag	UNP Q6D291
B	352	HIS	-	expression tag	UNP Q6D291

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Chain	Residue	Modelled	Actual	Comment	Reference
B	353	HIS	-	expression tag	UNP Q6D291
B	354	HIS	-	expression tag	UNP Q6D291
B	355	HIS	-	expression tag	UNP Q6D291
C	348	LEU	-	expression tag	UNP Q6D291
C	349	GLU	-	expression tag	UNP Q6D291
C	350	HIS	-	expression tag	UNP Q6D291
C	351	HIS	-	expression tag	UNP Q6D291
C	352	HIS	-	expression tag	UNP Q6D291
C	353	HIS	-	expression tag	UNP Q6D291
C	354	HIS	-	expression tag	UNP Q6D291
C	355	HIS	-	expression tag	UNP Q6D291
D	348	LEU	-	expression tag	UNP Q6D291
D	349	GLU	-	expression tag	UNP Q6D291
D	350	HIS	-	expression tag	UNP Q6D291
D	351	HIS	-	expression tag	UNP Q6D291
D	352	HIS	-	expression tag	UNP Q6D291
D	353	HIS	-	expression tag	UNP Q6D291
D	354	HIS	-	expression tag	UNP Q6D291
D	355	HIS	-	expression tag	UNP Q6D291
E	348	LEU	-	expression tag	UNP Q6D291
E	349	GLU	-	expression tag	UNP Q6D291
E	350	HIS	-	expression tag	UNP Q6D291
E	351	HIS	-	expression tag	UNP Q6D291
E	352	HIS	-	expression tag	UNP Q6D291
E	353	HIS	-	expression tag	UNP Q6D291
E	354	HIS	-	expression tag	UNP Q6D291
E	355	HIS	-	expression tag	UNP Q6D291
F	348	LEU	-	expression tag	UNP Q6D291
F	349	GLU	-	expression tag	UNP Q6D291
F	350	HIS	-	expression tag	UNP Q6D291
F	351	HIS	-	expression tag	UNP Q6D291
F	352	HIS	-	expression tag	UNP Q6D291
F	353	HIS	-	expression tag	UNP Q6D291
F	354	HIS	-	expression tag	UNP Q6D291
F	355	HIS	-	expression tag	UNP Q6D291
G	348	LEU	-	expression tag	UNP Q6D291
G	349	GLU	-	expression tag	UNP Q6D291
G	350	HIS	-	expression tag	UNP Q6D291
G	351	HIS	-	expression tag	UNP Q6D291
G	352	HIS	-	expression tag	UNP Q6D291
G	353	HIS	-	expression tag	UNP Q6D291
G	354	HIS	-	expression tag	UNP Q6D291

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Chain	Residue	Modelled	Actual	Comment	Reference
G	355	HIS	-	expression tag	UNP Q6D291
H	348	LEU	-	expression tag	UNP Q6D291
H	349	GLU	-	expression tag	UNP Q6D291
H	350	HIS	-	expression tag	UNP Q6D291
H	351	HIS	-	expression tag	UNP Q6D291
H	352	HIS	-	expression tag	UNP Q6D291
H	353	HIS	-	expression tag	UNP Q6D291
H	354	HIS	-	expression tag	UNP Q6D291
H	355	HIS	-	expression tag	UNP Q6D291

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	3	Total O 3 3	0	0
2	C	5	Total O 5 5	0	0
2	D	7	Total O 7 7	0	0
2	E	5	Total O 5 5	0	0
2	F	2	Total O 2 2	0	0
2	G	9	Total O 9 9	0	0
2	H	4	Total O 4 4	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.45Å 150.21Å 185.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.43 – 2.50 63.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.0 (63.43-2.50) 88.0 (63.43-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.218 , 0.248 0.221 , 0.249	Depositor DCC
$R_{free}$ test set	5077 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtrriage
Anisotropy	0.136	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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](#)

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	0.68	0/2781	0.92	17/3779 (0.4%)
1	B	0.66	0/2781	0.83	7/3779 (0.2%)
1	C	0.73	2/2781 (0.1%)	0.86	10/3779 (0.3%)
1	D	0.67	1/2781 (0.0%)	0.86	10/3779 (0.3%)
1	E	0.70	2/2781 (0.1%)	0.89	10/3779 (0.3%)
1	F	0.65	1/2781 (0.0%)	0.84	9/3779 (0.2%)
1	G	0.62	0/2781	0.82	4/3779 (0.1%)
1	H	0.74	3/2781 (0.1%)	0.90	12/3779 (0.3%)
All	All	0.68	9/22248 (0.0%)	0.87	79/30232 (0.3%)

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	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	H	0	2
All	All	0	10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	233	PRO	CA-C	10.92	1.74	1.52
1	C	235	VAL	N-CA	10.70	1.67	1.46
1	H	233	PRO	N-CA	8.77	1.62	1.47
1	E	234	GLY	N-CA	6.78	1.56	1.46
1	E	184	SER	CA-CB	-6.53	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	CYS	CB-SG	6.00	1.92	1.82
1	H	1	CYS	CB-SG	5.91	1.92	1.82
1	F	184	SER	CA-CB	-5.50	1.44	1.52
1	D	91	SER	CB-OG	-5.29	1.35	1.42

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH2	17.32	128.96	120.30
1	E	184	SER	C-N-CD	11.51	152.56	128.40
1	G	150	HIS	CB-CA-C	-11.24	87.91	110.40
1	F	184	SER	C-N-CD	10.76	150.99	128.40
1	D	276	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	D	276	ARG	CG-CD-NE	8.60	129.85	111.80
1	A	3	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	F	184	SER	C-N-CA	-8.18	87.65	122.00
1	A	209	THR	N-CA-C	8.08	132.82	111.00
1	E	184	SER	C-N-CA	-7.95	88.60	122.00
1	H	3	ARG	CG-CD-NE	7.71	127.99	111.80
1	A	146	LEU	CA-CB-CG	7.69	133.00	115.30
1	D	276	ARG	CB-CG-CD	-7.67	91.67	111.60
1	H	233	PRO	N-CA-C	7.55	131.74	112.10
1	E	31	LEU	CB-CG-CD1	7.44	123.65	111.00
1	E	184	SER	N-CA-C	7.43	131.07	111.00
1	F	184	SER	N-CA-C	7.22	130.50	111.00
1	H	145	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	G	3	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	3	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	H	233	PRO	CA-C-N	7.15	130.51	116.20
1	B	146	LEU	CA-CB-CG	6.74	130.80	115.30
1	H	233	PRO	O-C-N	-6.47	112.19	123.20
1	F	102	LYS	CD-CE-NZ	-6.41	96.95	111.70
1	H	233	PRO	C-N-CA	6.36	135.66	122.30
1	A	3	ARG	CG-CD-NE	6.32	125.06	111.80
1	C	1	CYS	N-CA-C	6.25	127.89	111.00
1	A	210	ASN	N-CA-CB	6.25	121.85	110.60
1	F	184	SER	CB-CA-C	-6.21	98.30	110.10
1	E	1	CYS	N-CA-C	6.11	127.51	111.00
1	E	184	SER	CB-CA-C	-6.07	98.57	110.10
1	E	67	LYS	CA-CB-CG	6.06	126.73	113.40
1	F	284	LYS	CB-CG-CD	6.05	127.32	111.60
1	A	218	ARG	NE-CZ-NH1	6.03	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	VAL	N-CA-CB	6.01	124.72	111.50
1	F	146	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	209	THR	CB-CA-C	-5.95	95.52	111.60
1	B	347	LEU	CA-CB-CG	5.91	128.90	115.30
1	H	337	LYS	CA-CB-CG	5.87	126.31	113.40
1	A	276	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	148	THR	N-CA-C	5.83	126.74	111.00
1	H	145	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	232	ILE	CB-CA-C	5.79	123.17	111.60
1	D	347	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	275	THR	N-CA-CB	5.61	120.96	110.30
1	A	211	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	66	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	19	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	148	THR	N-CA-C	-5.56	95.98	111.00
1	D	155	ASP	CB-CA-C	-5.56	99.28	110.40
1	E	155	ASP	CB-CA-C	-5.56	99.28	110.40
1	D	13	ASP	CB-CG-OD1	5.55	123.30	118.30
1	H	155	ASP	CB-CA-C	-5.52	99.36	110.40
1	G	218	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	F	218	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	155	ASP	CB-CA-C	-5.38	99.64	110.40
1	B	19	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	H	1	CYS	N-CA-C	5.35	125.44	111.00
1	C	155	ASP	CB-CA-C	-5.34	99.72	110.40
1	F	3	ARG	CG-CD-NE	5.33	122.98	111.80
1	A	3	ARG	CB-CG-CD	5.31	125.41	111.60
1	C	66	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	237	GLU	N-CA-CB	5.29	120.13	110.60
1	E	3	ARG	CG-CD-NE	5.27	122.87	111.80
1	A	19	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	218	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	218	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	148	THR	N-CA-C	5.16	124.93	111.00
1	E	199	GLN	CA-CB-CG	5.11	124.64	113.40
1	A	155	ASP	CB-CA-C	-5.11	100.19	110.40
1	C	3	ARG	CG-CD-NE	5.10	122.50	111.80
1	A	211	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	331	GLN	CB-CA-C	-5.05	100.29	110.40
1	H	138	LYS	CB-CG-CD	5.05	124.73	111.60
1	D	218	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	G	155	ASP	CB-CA-C	-5.04	100.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	218	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	218	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	140	VAL	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	GLY	Peptide
1	B	137	THR	Peptide
1	C	346	GLY	Peptide
1	D	1	CYS	Peptide
1	D	139	GLN	Peptide
1	E	183	ASN	Peptide
1	F	137	THR	Peptide
1	F	183	ASN	Peptide
1	H	101	LYS	Peptide
1	H	233	PRO	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2711	0	2660	72	0
1	B	2711	0	2660	43	0
1	C	2711	0	2660	30	18
1	D	2711	0	2658	44	18
1	E	2711	0	2660	27	13
1	F	2711	0	2659	22	0
1	G	2711	0	2660	27	0
1	H	2711	0	2660	39	13
2	A	11	0	0	2	0
2	B	3	0	0	0	0
2	C	5	0	0	2	0
2	D	7	0	0	4	0
2	E	5	0	0	0	0
2	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	9	0	0	1	0
2	H	4	0	0	0	0
All	All	21734	0	21277	291	31

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 7.

All (291) 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:235:VAL:N	1:C:235:VAL:CA	1.67	1.56
1:H:233:PRO:CA	1:H:233:PRO:C	1.74	1.54
1:D:68:GLY:O	1:D:138:LYS:NZ	1.57	1.34
1:A:3:ARG:NH1	1:A:181:MET:SD	2.03	1.31
1:B:209:THR:HG22	1:B:214:ASP:OD2	1.21	1.28
1:D:25:ASP:C	1:D:276:ARG:HH21	1.37	1.26
1:D:26:ASP:N	1:D:276:ARG:HH21	1.36	1.21
1:D:1:CYS:HB3	2:D:406:HOH:O	1.42	1.19
1:A:300:TRP:NE1	1:A:331:GLN:OE1	1.74	1.17
1:B:209:THR:CG2	1:B:214:ASP:OD2	1.94	1.15
1:C:71:SER:O	2:C:404:HOH:O	1.64	1.14
1:A:276:ARG:HG3	1:A:276:ARG:NH1	1.57	1.10
1:A:23:TRP:N	1:A:276:ARG:HH12	1.49	1.10
1:D:25:ASP:C	1:D:276:ARG:NH2	2.11	1.03
1:A:3:ARG:NH1	1:A:181:MET:CE	2.24	1.00
1:D:138:LYS:HE2	1:D:140:VAL:HG11	1.44	0.99
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.21	0.99
1:A:240:LYS:HD2	2:A:409:HOH:O	1.65	0.97
1:H:302:ASP:HB2	1:H:331:GLN:HE21	1.29	0.96
1:A:23:TRP:N	1:A:276:ARG:NH1	2.16	0.94
1:D:26:ASP:N	1:D:276:ARG:NH2	2.15	0.93
1:A:27:THR:OG1	1:A:29:THR:HG22	1.69	0.91
1:A:300:TRP:CD1	1:A:331:GLN:NE2	2.38	0.91
1:A:260:VAL:H	1:A:275:THR:CG2	1.82	0.91
1:A:276:ARG:CG	1:A:276:ARG:HH11	1.80	0.90
1:A:23:TRP:H	1:A:276:ARG:NH1	1.68	0.89
1:A:331:GLN:HA	1:A:331:GLN:NE2	1.88	0.87
1:A:29:THR:HB	1:A:61:SER:O	1.74	0.87
1:D:1:CYS:CB	2:D:406:HOH:O	2.10	0.86
1:F:204:VAL:HG13	1:G:204:VAL:HG13	1.57	0.86
1:D:140:VAL:HG13	1:D:140:VAL:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TRP:HB3	1:A:276:ARG:CZ	2.04	0.86
1:E:204:VAL:O	1:F:211:ARG:NH2	2.07	0.86
1:A:23:TRP:H	1:A:276:ARG:HH12	0.86	0.86
1:E:211:ARG:NH2	1:F:204:VAL:O	2.08	0.85
1:D:27:THR:HG23	1:D:29:THR:OG1	1.76	0.85
1:A:3:ARG:HH12	1:A:181:MET:CE	1.86	0.85
1:A:21:MET:HG3	1:A:276:ARG:NH2	1.93	0.83
1:H:233:PRO:HA	1:H:233:PRO:C	1.94	0.83
1:B:204:VAL:O	1:C:211:ARG:NH2	2.11	0.82
1:A:22:ASP:C	1:A:276:ARG:HH22	1.84	0.81
1:A:23:TRP:CB	1:A:276:ARG:CZ	2.58	0.81
1:H:220:SER:O	1:H:224:LYS:HD2	1.80	0.80
1:A:23:TRP:HB2	1:A:276:ARG:NH2	1.97	0.79
1:A:29:THR:HG21	1:A:277:TRP:NE1	1.95	0.79
1:H:63:PHE:HB2	1:H:69:MET:O	1.82	0.79
1:B:141:GLU:HB2	1:B:144:LYS:HD3	1.65	0.78
1:D:204:VAL:O	1:G:211:ARG:NH2	2.16	0.78
1:D:139:GLN:HB2	1:D:140:VAL:HA	1.66	0.78
1:D:1:CYS:CA	2:D:406:HOH:O	2.29	0.78
1:D:204:VAL:HG13	1:E:204:VAL:HG13	1.66	0.77
1:H:302:ASP:HB2	1:H:331:GLN:NE2	1.99	0.77
1:B:141:GLU:OE2	1:B:144:LYS:NZ	2.17	0.77
1:C:140:VAL:HG23	1:C:140:VAL:O	1.86	0.76
1:E:184:SER:CB	1:E:212:ALA:CB	2.65	0.75
1:D:1:CYS:N	1:D:86:LEU:HG	2.02	0.74
1:F:184:SER:CB	1:F:212:ALA:CB	2.65	0.74
1:H:43:GLY:O	1:H:44:ALA:HB2	1.88	0.73
1:A:21:MET:HG3	1:A:276:ARG:HH21	1.52	0.72
1:E:138:LYS:HE2	1:E:140:VAL:HG22	1.71	0.72
1:B:139:GLN:HG3	1:B:141:GLU:HB3	1.71	0.71
1:B:107:VAL:HG22	1:B:149:LEU:HD11	1.71	0.71
1:D:211:ARG:NH2	1:G:204:VAL:O	2.22	0.71
1:C:204:VAL:HG13	1:H:204:VAL:HG13	1.73	0.71
1:D:69:MET:SD	1:D:141:GLU:HG2	2.32	0.70
1:E:107:VAL:HG22	1:E:149:LEU:HD11	1.74	0.70
1:H:102:LYS:CE	1:H:131:GLU:O	2.41	0.69
1:D:138:LYS:HE2	1:D:140:VAL:CG1	2.20	0.69
1:A:21:MET:CG	1:A:276:ARG:HH21	2.04	0.69
1:A:29:THR:HG21	1:A:277:TRP:HE1	1.56	0.69
1:A:22:ASP:OD2	1:A:275:THR:HB	1.92	0.69
1:A:260:VAL:H	1:A:275:THR:HG23	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:VAL:HG22	1:F:149:LEU:HD11	1.74	0.69
1:B:141:GLU:CD	1:B:144:LYS:NZ	2.46	0.69
1:C:143:GLN:HG3	1:C:145:ARG:H	1.58	0.68
1:A:3:ARG:HH12	1:A:181:MET:HE1	1.58	0.68
1:C:62:ALA:O	2:C:404:HOH:O	2.11	0.68
1:G:107:VAL:HG22	1:G:149:LEU:HD11	1.74	0.68
1:D:1:CYS:H1	1:D:86:LEU:HG	1.58	0.67
1:G:141:GLU:OE2	1:G:141:GLU:HA	1.92	0.67
1:A:23:TRP:CB	1:A:276:ARG:NH2	2.57	0.67
1:A:23:TRP:O	1:A:276:ARG:NH1	2.28	0.67
1:H:102:LYS:HE2	1:H:131:GLU:O	1.94	0.67
1:A:300:TRP:NE1	1:A:331:GLN:CD	2.47	0.67
1:E:1:CYS:SG	1:E:22:ASP:HB2	2.35	0.67
1:A:140:VAL:HG21	1:A:146:LEU:HD11	1.77	0.66
1:E:138:LYS:CE	1:E:140:VAL:HG22	2.26	0.66
1:E:184:SER:CB	1:E:212:ALA:HB1	2.25	0.66
1:D:25:ASP:CA	1:D:276:ARG:NH2	2.59	0.66
1:C:235:VAL:N	1:C:235:VAL:C	2.49	0.65
1:B:95:LYS:HE3	1:B:95:LYS:HA	1.77	0.65
1:F:184:SER:CB	1:F:212:ALA:HB1	2.27	0.65
1:E:138:LYS:HE2	1:E:140:VAL:CG2	2.27	0.64
1:F:137:THR:O	1:F:138:LYS:HB2	1.98	0.64
1:D:141:GLU:OE1	1:D:141:GLU:HA	1.98	0.64
1:A:27:THR:OG1	1:A:29:THR:CG2	2.44	0.64
1:B:141:GLU:CD	1:B:144:LYS:HZ1	1.98	0.64
1:C:140:VAL:CG2	1:C:140:VAL:O	2.46	0.63
1:D:27:THR:CG2	1:D:29:THR:OG1	2.44	0.63
1:H:1:CYS:SG	1:H:22:ASP:HB2	2.38	0.63
1:A:204:VAL:HG13	1:B:204:VAL:HG13	1.80	0.63
1:D:140:VAL:CG1	1:D:140:VAL:O	2.45	0.63
1:G:142:GLY:HA3	1:G:143:GLN:HG3	1.81	0.62
1:H:47:TYR:CD2	1:H:99:THR:HA	2.34	0.62
1:D:138:LYS:NZ	1:D:140:VAL:HG12	2.14	0.62
1:E:184:SER:HB2	1:E:212:ALA:CB	2.30	0.62
1:E:184:SER:HB2	1:E:212:ALA:HB1	1.80	0.62
1:F:143:GLN:HG3	1:F:143:GLN:O	2.00	0.62
1:F:184:SER:HB2	1:F:212:ALA:HB1	1.82	0.61
1:B:209:THR:CG2	1:B:214:ASP:CG	2.68	0.60
1:A:260:VAL:H	1:A:275:THR:HG22	1.64	0.60
1:F:184:SER:HB2	1:F:212:ALA:CB	2.31	0.60
1:H:47:TYR:CD2	1:H:100:ALA:N	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:CD	2:A:409:HOH:O	2.37	0.59
1:D:97:LYS:HG3	1:D:98:PRO:HD2	1.82	0.59
1:H:101:LYS:HA	1:H:103:PRO:HD3	1.83	0.59
1:A:23:TRP:CA	1:A:276:ARG:NH1	2.65	0.59
1:C:1:CYS:SG	1:C:22:ASP:HB2	2.42	0.58
1:G:138:LYS:HG3	1:G:347:LEU:HD23	1.84	0.58
1:G:92:GLU:OE1	1:G:167:ASP:N	2.22	0.58
1:H:209:THR:HG22	1:H:211:ARG:H	1.69	0.58
1:C:140:VAL:HG12	1:C:147:ALA:HB2	1.84	0.58
1:D:27:THR:HG21	1:D:277:TRP:HE1	1.69	0.58
1:B:139:GLN:HG3	1:B:141:GLU:CB	2.35	0.57
1:A:3:ARG:CZ	1:A:181:MET:SD	2.90	0.56
1:H:155:ASP:HB3	1:H:157:SER:H	1.70	0.56
1:B:47:TYR:CD2	1:B:99:THR:HA	2.41	0.56
1:F:137:THR:O	1:F:138:LYS:CB	2.52	0.56
1:G:139:GLN:O	1:G:145:ARG:CZ	2.54	0.56
1:F:155:ASP:HB3	1:F:157:SER:H	1.70	0.56
1:A:145:ARG:C	1:A:146:LEU:HD22	2.26	0.55
1:A:23:TRP:N	1:A:276:ARG:CZ	2.69	0.55
1:B:145:ARG:O	1:B:146:LEU:HD12	2.07	0.55
1:D:135:LEU:HD12	1:D:165:TYR:CE1	2.42	0.55
1:G:155:ASP:HB3	1:G:157:SER:H	1.70	0.55
1:A:3:ARG:HH21	1:A:5:VAL:HG23	1.72	0.55
1:G:138:LYS:HG3	1:G:347:LEU:CD2	2.37	0.55
1:C:155:ASP:HB3	1:C:157:SER:H	1.72	0.54
1:C:209:THR:O	1:C:218:ARG:NH2	2.40	0.54
1:B:209:THR:OG1	1:B:210:ASN:N	2.41	0.54
1:D:139:GLN:HB2	1:D:140:VAL:CA	2.38	0.54
1:D:139:GLN:CB	1:D:140:VAL:HA	2.36	0.54
1:D:209:THR:O	1:D:218:ARG:NH2	2.41	0.54
1:A:23:TRP:N	1:A:276:ARG:HH22	2.06	0.54
1:A:21:MET:SD	1:A:276:ARG:NH2	2.80	0.54
1:B:141:GLU:OE1	1:B:142:GLY:N	2.40	0.54
1:H:137:THR:HG23	1:H:138:LYS:CG	2.37	0.54
1:F:209:THR:O	1:F:218:ARG:NH2	2.41	0.54
1:A:300:TRP:CE2	1:A:331:GLN:OE1	2.57	0.54
1:C:45:GLY:N	1:C:347:LEU:C	2.61	0.53
1:G:102:LYS:HD2	1:G:134:ILE:HG12	1.90	0.53
1:E:135:LEU:HD12	1:E:165:TYR:CE1	2.43	0.53
1:E:209:THR:O	1:E:218:ARG:NH2	2.42	0.53
1:A:229:ASN:OD1	1:A:238:LYS:HE3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASN:OD1	1:C:238:LYS:HE3	2.09	0.53
1:B:144:LYS:HB2	1:B:145:ARG:HA	1.90	0.53
1:G:209:THR:O	1:G:218:ARG:NH2	2.41	0.53
1:F:229:ASN:OD1	1:F:238:LYS:HE3	2.09	0.52
1:A:140:VAL:CG2	1:A:146:LEU:HD11	2.39	0.52
1:B:229:ASN:OD1	1:B:238:LYS:HE3	2.09	0.52
1:G:229:ASN:OD1	1:G:238:LYS:HE3	2.09	0.52
1:B:47:TYR:HD2	1:B:99:THR:HA	1.73	0.52
1:B:197:TRP:O	1:B:200:ILE:O	2.28	0.52
1:H:209:THR:HB	1:H:214:ASP:OD2	2.10	0.52
1:A:155:ASP:HB3	1:A:157:SER:H	1.74	0.52
1:A:259:SER:HB3	1:A:275:THR:CG2	2.40	0.52
1:B:135:LEU:HD12	1:B:165:TYR:CE1	2.44	0.52
1:D:1:CYS:C	2:D:406:HOH:O	2.45	0.52
1:A:3:ARG:NH1	1:A:181:MET:HE1	2.15	0.52
1:B:155:ASP:HB3	1:B:157:SER:H	1.74	0.51
1:B:209:THR:O	1:B:218:ARG:NH2	2.43	0.51
1:E:229:ASN:OD1	1:E:238:LYS:HE3	2.10	0.51
1:G:197:TRP:O	1:G:200:ILE:O	2.28	0.51
1:H:197:TRP:O	1:H:200:ILE:O	2.29	0.51
1:H:209:THR:O	1:H:218:ARG:NH2	2.44	0.51
1:A:197:TRP:O	1:A:200:ILE:O	2.28	0.51
1:B:145:ARG:O	1:B:145:ARG:HG2	2.09	0.51
1:D:197:TRP:O	1:D:200:ILE:O	2.28	0.51
1:D:229:ASN:OD1	1:D:238:LYS:HE3	2.09	0.51
1:C:197:TRP:O	1:C:200:ILE:O	2.29	0.51
1:A:23:TRP:N	1:A:276:ARG:NH2	2.58	0.51
1:H:135:LEU:HD12	1:H:165:TYR:CE1	2.45	0.51
1:F:197:TRP:O	1:F:200:ILE:O	2.28	0.51
1:B:138:LYS:HG3	1:B:139:GLN:N	2.26	0.51
1:E:197:TRP:O	1:E:200:ILE:O	2.28	0.51
1:D:155:ASP:HB3	1:D:157:SER:H	1.76	0.51
1:F:138:LYS:HG3	1:F:139:GLN:N	2.26	0.50
1:D:138:LYS:CE	1:D:140:VAL:CG1	2.87	0.50
1:H:240:LYS:NZ	1:H:244:ASP:OD1	2.42	0.50
1:E:9:PRO:HD2	1:E:227:ASN:ND2	2.27	0.50
1:A:298:ILE:HG22	1:H:298:ILE:HG22	1.94	0.49
1:G:140:VAL:O	1:G:141:GLU:HG2	2.12	0.49
1:D:1:CYS:HB2	1:D:20:SER:O	2.13	0.49
1:F:146:LEU:HD23	1:F:148:THR:OG1	2.11	0.49
1:G:240:LYS:NZ	1:G:244:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:LYS:HD2	1:E:134:ILE:HG12	1.95	0.49
1:A:300:TRP:NE1	1:A:331:GLN:NE2	2.60	0.48
1:D:268:ASP:OD1	1:D:268:ASP:N	2.46	0.48
1:A:140:VAL:CB	1:A:146:LEU:HD11	2.44	0.48
1:B:232:ILE:HB	1:B:235:VAL:HG13	1.96	0.47
1:E:240:LYS:NZ	1:E:244:ASP:OD1	2.43	0.47
1:B:144:LYS:CB	1:B:145:ARG:HA	2.43	0.47
1:D:298:ILE:HG22	1:G:298:ILE:HG22	1.96	0.47
1:E:155:ASP:HB3	1:E:157:SER:H	1.80	0.47
1:H:137:THR:HG23	1:H:138:LYS:HG3	1.96	0.47
1:H:63:PHE:CB	1:H:69:MET:O	2.56	0.47
1:B:95:LYS:HA	1:B:95:LYS:CE	2.39	0.47
1:D:1:CYS:H2	1:D:86:LEU:HG	1.76	0.47
1:F:19:ARG:NH2	1:F:85:VAL:O	2.47	0.47
1:A:260:VAL:N	1:A:275:THR:HG23	2.28	0.47
1:A:209:THR:O	1:A:210:ASN:CB	2.63	0.47
1:A:259:SER:HB3	1:A:275:THR:HG23	1.97	0.47
1:A:145:ARG:O	1:A:146:LEU:HD22	2.15	0.47
1:G:138:LYS:HE3	1:G:347:LEU:HA	1.97	0.47
1:B:169:LYS:HD2	1:B:169:LYS:N	2.31	0.46
1:B:46:GLN:OE1	1:B:47:TYR:CE1	2.69	0.46
1:C:140:VAL:CG2	1:C:145:ARG:HE	2.29	0.46
1:B:232:ILE:O	1:B:235:VAL:HG13	2.16	0.46
1:C:237:GLU:HG3	1:C:238:LYS:O	2.15	0.46
1:E:1:CYS:HB2	1:E:22:ASP:CG	2.36	0.46
1:H:69:MET:HG3	1:H:69:MET:O	2.16	0.46
1:A:259:SER:CB	1:A:275:THR:HG21	2.46	0.46
1:D:138:LYS:NZ	1:D:140:VAL:CG1	2.78	0.46
1:B:145:ARG:O	1:B:145:ARG:CG	2.63	0.46
1:A:102:LYS:HD3	1:A:102:LYS:HA	1.60	0.45
1:D:240:LYS:NZ	1:D:244:ASP:OD1	2.42	0.45
1:H:19:ARG:NH2	1:H:85:VAL:O	2.48	0.45
1:A:143:GLN:HA	1:A:144:LYS:HA	1.81	0.45
1:C:45:GLY:H	1:C:347:LEU:C	2.19	0.45
1:G:19:ARG:NH2	1:G:85:VAL:O	2.49	0.45
1:H:47:TYR:CD2	1:H:99:THR:CA	3.00	0.45
1:E:1:CYS:HB2	1:E:22:ASP:OD1	2.17	0.45
1:H:47:TYR:HD2	1:H:99:THR:HA	1.78	0.45
1:B:209:THR:HG23	1:B:214:ASP:CG	2.38	0.45
1:A:29:THR:CG2	1:A:277:TRP:HE1	2.27	0.44
1:C:141:GLU:HA	1:C:142:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:VAL:O	1:G:141:GLU:CB	2.65	0.44
1:A:260:VAL:N	1:A:275:THR:CG2	2.66	0.44
1:B:284:LYS:HA	1:B:284:LYS:HD3	1.83	0.44
1:E:231:LEU:O	1:E:232:ILE:HD13	2.17	0.44
1:D:146:LEU:HA	1:D:146:LEU:HD12	1.75	0.44
1:F:240:LYS:NZ	1:F:244:ASP:OD1	2.44	0.44
1:C:19:ARG:NH2	1:C:85:VAL:O	2.50	0.44
1:B:240:LYS:NZ	1:B:244:ASP:OD1	2.43	0.44
1:F:143:GLN:O	1:F:143:GLN:CG	2.65	0.44
1:G:142:GLY:HA2	1:G:145:ARG:HH21	1.83	0.43
1:G:225:ASN:HB3	2:G:408:HOH:O	2.17	0.43
1:C:140:VAL:HG21	1:C:145:ARG:HE	1.83	0.43
1:H:1:CYS:HB2	1:H:22:ASP:CG	2.39	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.78	0.43
1:B:192:THR:OG1	1:H:195:ALA:HB1	2.18	0.43
1:H:147:ALA:C	1:H:148:THR:OG1	2.56	0.43
1:H:1:CYS:HB2	1:H:22:ASP:OD1	2.18	0.43
1:C:233:PRO:HA	1:C:234:GLY:HA2	1.67	0.42
1:F:145:ARG:HB2	1:F:146:LEU:HD13	2.01	0.42
1:A:21:MET:CG	1:A:276:ARG:NH2	2.66	0.42
1:C:14:TYR:OH	1:C:282:ASP:OD2	2.29	0.42
1:G:23:TRP:O	1:G:276:ARG:HD2	2.20	0.42
1:C:68:GLY:O	1:C:138:LYS:HE2	2.20	0.42
1:H:3:ARG:HG2	1:H:4:PHE:N	2.35	0.42
1:C:138:LYS:HB3	1:C:138:LYS:HE3	1.79	0.42
1:E:23:TRP:O	1:E:276:ARG:HD2	2.18	0.42
1:G:143:GLN:HA	1:G:144:LYS:HA	1.85	0.42
1:H:233:PRO:CB	1:H:233:PRO:C	2.78	0.42
1:A:142:GLY:O	1:A:143:GLN:HB2	2.19	0.42
1:H:302:ASP:CB	1:H:331:GLN:NE2	2.78	0.42
1:B:139:GLN:CG	1:B:144:LYS:HE3	2.50	0.41
1:B:47:TYR:HD2	1:B:99:THR:CA	2.32	0.41
1:A:259:SER:HA	1:A:275:THR:HG21	2.01	0.41
1:A:300:TRP:CD1	1:A:331:GLN:CD	2.88	0.41
1:E:282:ASP:C	1:E:282:ASP:OD1	2.58	0.41
1:G:138:LYS:CG	1:G:139:GLN:H	2.33	0.41
1:H:300:TRP:HE1	1:H:331:GLN:NE2	2.18	0.41
1:D:1:CYS:H1	1:D:86:LEU:CG	2.28	0.41
1:B:232:ILE:HB	1:B:235:VAL:CG1	2.50	0.41
1:F:302:ASP:H	1:F:331:GLN:NE2	2.18	0.41
1:B:192:THR:OG1	1:H:195:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:NZ	1:C:244:ASP:OD1	2.43	0.41
1:D:25:ASP:HA	1:D:276:ARG:NH2	2.31	0.41
1:E:1:CYS:HB2	1:E:22:ASP:HB2	2.03	0.41
1:H:44:ALA:HA	1:H:45:GLY:HA2	1.77	0.41
1:G:284:LYS:HD3	1:G:284:LYS:HA	1.87	0.41
1:E:31:LEU:HB2	1:E:318:LEU:HB3	2.02	0.41
1:B:144:LYS:HZ3	1:B:146:LEU:N	2.18	0.41
1:A:29:THR:CG2	1:A:277:TRP:NE1	2.76	0.40
1:A:44:ALA:O	1:A:48:SER:HB3	2.21	0.40
1:C:30:ASN:ND2	1:C:320:LEU:H	2.19	0.40
1:B:23:TRP:O	1:B:276:ARG:HD2	2.20	0.40
1:C:282:ASP:C	1:C:282:ASP:OD1	2.60	0.40
1:A:44:ALA:H	1:A:48:SER:HB2	1.87	0.40
1:C:284:LYS:HA	1:C:284:LYS:HD3	1.90	0.40

All (31) 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:C:235:VAL:N	1:D:234:GLY:C[4_555]	0.89	1.31
1:C:235:VAL:N	1:D:234:GLY:CA[4_555]	1.01	1.19
1:C:234:GLY:O	1:D:234:GLY:O[4_555]	1.05	1.15
1:E:233:PRO:C	1:H:233:PRO:N[4_455]	1.06	1.14
1:E:233:PRO:O	1:H:233:PRO:N[4_455]	1.13	1.07
1:E:232:ILE:O	1:H:233:PRO:O[4_455]	1.22	0.98
1:C:234:GLY:C	1:D:234:GLY:C[4_555]	1.32	0.88
1:C:234:GLY:N	1:D:233:PRO:O[4_555]	1.54	0.66
1:E:233:PRO:O	1:H:233:PRO:CB[4_455]	1.57	0.63
1:C:235:VAL:N	1:D:235:VAL:N[4_555]	1.60	0.60
1:C:234:GLY:C	1:D:234:GLY:O[4_555]	1.64	0.56
1:E:232:ILE:O	1:H:234:GLY:N[4_455]	1.70	0.50
1:C:233:PRO:O	1:D:233:PRO:O[4_555]	1.71	0.49
1:E:234:GLY:N	1:H:232:ILE:O[4_455]	1.71	0.49
1:E:233:PRO:O	1:H:233:PRO:CG[4_455]	1.73	0.47
1:C:234:GLY:O	1:D:234:GLY:C[4_555]	1.74	0.46
1:C:235:VAL:C	1:D:234:GLY:O[4_555]	1.76	0.44
1:E:234:GLY:N	1:H:233:PRO:N[4_455]	1.80	0.40
1:C:235:VAL:N	1:D:234:GLY:N[4_555]	1.81	0.39
1:C:235:VAL:CA	1:D:234:GLY:CA[4_555]	1.82	0.38
1:E:233:PRO:C	1:H:232:ILE:C[4_455]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLY:C	1:D:234:GLY:CA[4_555]	1.92	0.28
1:E:234:GLY:N	1:H:232:ILE:C[4_455]	1.93	0.27
1:C:235:VAL:CA	1:D:235:VAL:N[4_555]	1.97	0.23
1:C:235:VAL:C	1:D:234:GLY:C[4_555]	1.98	0.22
1:C:235:VAL:N	1:D:234:GLY:O[4_555]	2.03	0.17
1:E:233:PRO:C	1:H:233:PRO:C[4_455]	2.09	0.11
1:C:236:ALA:N	1:D:234:GLY:O[4_555]	2.10	0.10
1:E:234:GLY:CA	1:H:233:PRO:CA[4_455]	2.13	0.07
1:E:232:ILE:C	1:H:233:PRO:O[4_455]	2.16	0.04
1:C:234:GLY:C	1:D:235:VAL:N[4_555]	2.19	0.01

## 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	345/355 (97%)	334 (97%)	8 (2%)	3 (1%)	17	31
1	B	345/355 (97%)	336 (97%)	7 (2%)	2 (1%)	25	43
1	C	345/355 (97%)	338 (98%)	6 (2%)	1 (0%)	41	61
1	D	345/355 (97%)	338 (98%)	7 (2%)	0	100	100
1	E	345/355 (97%)	337 (98%)	6 (2%)	2 (1%)	25	43
1	F	345/355 (97%)	336 (97%)	7 (2%)	2 (1%)	25	43
1	G	345/355 (97%)	337 (98%)	7 (2%)	1 (0%)	41	61
1	H	345/355 (97%)	332 (96%)	11 (3%)	2 (1%)	25	43
All	All	2760/2840 (97%)	2688 (97%)	59 (2%)	13 (0%)	29	48

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	ALA
1	H	138	LYS

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Mol	Chain	Res	Type
1	H	44	ALA
1	A	143	GLN
1	A	210	ASN
1	B	138	LYS
1	C	235	VAL
1	G	141	GLU
1	A	146	LEU
1	E	184	SER
1	F	184	SER
1	F	185	PRO
1	E	185	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/297 (97%)	272 (94%)	17 (6%)	19	37
1	B	289/297 (97%)	268 (93%)	21 (7%)	14	27
1	C	289/297 (97%)	272 (94%)	17 (6%)	19	37
1	D	289/297 (97%)	270 (93%)	19 (7%)	16	32
1	E	289/297 (97%)	264 (91%)	25 (9%)	10	20
1	F	289/297 (97%)	270 (93%)	19 (7%)	16	32
1	G	289/297 (97%)	271 (94%)	18 (6%)	18	35
1	H	289/297 (97%)	271 (94%)	18 (6%)	18	35
All	All	2312/2376 (97%)	2158 (93%)	154 (7%)	16	31

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	29	THR
1	A	66	ARG
1	A	84	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	86	LEU
1	A	90	GLU
1	A	92	GLU
1	A	95	LYS
1	A	102	LYS
1	A	138	LYS
1	A	141	GLU
1	A	145	ARG
1	A	146	LEU
1	A	148	THR
1	A	218	ARG
1	A	275	THR
1	A	347	LEU
1	B	3	ARG
1	B	19	ARG
1	B	46	GLN
1	B	67	LYS
1	B	84	ASN
1	B	92	GLU
1	B	95	LYS
1	B	97	LYS
1	B	107	VAL
1	B	135	LEU
1	B	138	LYS
1	B	141	GLU
1	B	144	LYS
1	B	145	ARG
1	B	146	LEU
1	B	148	THR
1	B	169	LYS
1	B	209	THR
1	B	235	VAL
1	B	276	ARG
1	B	347	LEU
1	C	3	ARG
1	C	19	ARG
1	C	46	GLN
1	C	66	ARG
1	C	67	LYS
1	C	84	ASN
1	C	86	LEU
1	C	92	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	97	LYS
1	C	141	GLU
1	C	144	LYS
1	C	145	ARG
1	C	146	LEU
1	C	148	THR
1	C	167	ASP
1	C	276	ARG
1	C	347	LEU
1	D	3	ARG
1	D	19	ARG
1	D	27	THR
1	D	46	GLN
1	D	66	ARG
1	D	84	ASN
1	D	86	LEU
1	D	91	SER
1	D	95	LYS
1	D	101	LYS
1	D	135	LEU
1	D	141	GLU
1	D	145	ARG
1	D	146	LEU
1	D	148	THR
1	D	268	ASP
1	D	276	ARG
1	D	337	LYS
1	D	347	LEU
1	E	3	ARG
1	E	19	ARG
1	E	31	LEU
1	E	46	GLN
1	E	66	ARG
1	E	84	ASN
1	E	90	GLU
1	E	92	GLU
1	E	95	LYS
1	E	102	LYS
1	E	107	VAL
1	E	126	LYS
1	E	135	LEU
1	E	139	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	140	VAL
1	E	141	GLU
1	E	143	GLN
1	E	144	LYS
1	E	146	LEU
1	E	148	THR
1	E	199	GLN
1	E	268	ASP
1	E	276	ARG
1	E	337	LYS
1	E	347	LEU
1	F	3	ARG
1	F	19	ARG
1	F	66	ARG
1	F	67	LYS
1	F	84	ASN
1	F	86	LEU
1	F	99	THR
1	F	101	LYS
1	F	102	LYS
1	F	107	VAL
1	F	138	LYS
1	F	140	VAL
1	F	141	GLU
1	F	145	ARG
1	F	146	LEU
1	F	148	THR
1	F	276	ARG
1	F	284	LYS
1	F	331	GLN
1	G	3	ARG
1	G	19	ARG
1	G	46	GLN
1	G	66	ARG
1	G	67	LYS
1	G	84	ASN
1	G	86	LEU
1	G	92	GLU
1	G	95	LYS
1	G	101	LYS
1	G	102	LYS
1	G	107	VAL

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Mol	Chain	Res	Type
1	G	143	GLN
1	G	144	LYS
1	G	145	ARG
1	G	148	THR
1	G	276	ARG
1	G	343	GLU
1	H	3	ARG
1	H	19	ARG
1	H	66	ARG
1	H	67	LYS
1	H	84	ASN
1	H	92	GLU
1	H	95	LYS
1	H	97	LYS
1	H	135	LEU
1	H	141	GLU
1	H	148	THR
1	H	209	THR
1	H	224	LYS
1	H	276	ARG
1	H	329	SER
1	H	331	GLN
1	H	337	LYS
1	H	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	225	ASN
1	B	340	GLN
1	C	30	ASN
1	C	84	ASN
1	C	179	GLN
1	D	139	GLN
1	E	340	GLN
1	F	210	ASN
1	F	331	GLN
1	G	36	GLN
1	H	36	GLN
1	H	179	GLN
1	H	331	GLN

### 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](#)

There are no ligands in this entry.

### 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	347/355 (97%)	0.17	12 (3%) 44 47	19, 34, 75, 172	0
1	B	347/355 (97%)	0.21	11 (3%) 47 51	18, 36, 77, 175	0
1	C	347/355 (97%)	0.07	12 (3%) 44 47	20, 34, 73, 201	0
1	D	347/355 (97%)	0.01	6 (1%) 70 72	18, 33, 69, 128	0
1	E	347/355 (97%)	0.19	16 (4%) 32 34	18, 34, 81, 182	0
1	F	347/355 (97%)	0.31	19 (5%) 25 26	20, 39, 83, 163	0
1	G	347/355 (97%)	0.19	12 (3%) 44 47	21, 39, 75, 199	0
1	H	347/355 (97%)	0.48	33 (9%) 8 8	21, 41, 86, 149	0
All	All	2776/2840 (97%)	0.20	121 (4%) 34 37	18, 36, 80, 201	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	143	GLN	14.6
1	G	144	LYS	13.9
1	A	140	VAL	13.6
1	F	141	GLU	13.4
1	H	143	GLN	13.4
1	E	140	VAL	13.4
1	A	143	GLN	13.1
1	H	144	LYS	12.9
1	B	141	GLU	10.7
1	H	139	GLN	10.4
1	D	140	VAL	10.1
1	A	142	GLY	10.0
1	E	143	GLN	9.7
1	B	140	VAL	9.7
1	B	145	ARG	9.6
1	H	141	GLU	8.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	142	GLY	8.5
1	C	233	PRO	8.5
1	A	147	ALA	8.5
1	H	140	VAL	8.4
1	H	142	GLY	8.3
1	B	144	LYS	8.2
1	G	139	GLN	7.9
1	G	145	ARG	7.0
1	C	236	ALA	6.9
1	B	142	GLY	6.9
1	F	45	GLY	6.8
1	H	145	ARG	6.7
1	F	139	GLN	6.6
1	E	233	PRO	6.6
1	A	141	GLU	6.6
1	H	147	ALA	6.5
1	E	141	GLU	6.4
1	G	140	VAL	6.2
1	F	144	LYS	6.2
1	C	231	LEU	6.2
1	B	143	GLN	6.1
1	A	146	LEU	6.0
1	B	146	LEU	6.0
1	H	44	ALA	6.0
1	C	235	VAL	5.9
1	E	144	LYS	5.9
1	B	139	GLN	5.8
1	C	232	ILE	5.7
1	A	144	LYS	5.7
1	F	143	GLN	5.5
1	F	140	VAL	5.4
1	F	142	GLY	5.4
1	F	147	ALA	5.4
1	E	146	LEU	5.1
1	D	233	PRO	5.0
1	D	347	LEU	4.8
1	E	145	ARG	4.8
1	E	142	GLY	4.6
1	G	146	LEU	4.4
1	H	137	THR	4.2
1	H	233	PRO	4.2
1	G	147	ALA	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	347	LEU	3.9
1	A	139	GLN	3.8
1	A	145	ARG	3.7
1	E	1	CYS	3.7
1	H	138	LYS	3.6
1	H	135	LEU	3.6
1	F	104	GLY	3.5
1	C	234	GLY	3.5
1	F	166	ILE	3.4
1	F	145	ARG	3.4
1	F	184	SER	3.4
1	F	146	LEU	3.4
1	H	42	GLY	3.3
1	H	346	GLY	3.2
1	C	141	GLU	3.2
1	E	139	GLN	3.2
1	H	146	LEU	3.2
1	B	147	ALA	3.1
1	G	141	GLU	3.1
1	D	232	ILE	3.0
1	E	69	MET	3.0
1	H	101	LYS	3.0
1	F	346	GLY	2.9
1	E	234	GLY	2.9
1	C	237	GLU	2.9
1	H	69	MET	2.8
1	H	45	GLY	2.8
1	H	93	TYR	2.8
1	A	276	ARG	2.8
1	H	104	GLY	2.8
1	H	234	GLY	2.8
1	B	67	LYS	2.7
1	B	68	GLY	2.7
1	F	167	ASP	2.6
1	D	235	VAL	2.6
1	G	347	LEU	2.6
1	E	232	ILE	2.5
1	G	45	GLY	2.5
1	H	96	THR	2.5
1	H	136	VAL	2.5
1	F	69	MET	2.5
1	C	1	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	140	VAL	2.4
1	H	232	ILE	2.3
1	H	97	LYS	2.3
1	E	147	ALA	2.3
1	G	93	TYR	2.3
1	H	41	SER	2.3
1	F	133	PHE	2.3
1	F	47	TYR	2.3
1	H	91	SER	2.2
1	H	345	ALA	2.2
1	E	269	MET	2.2
1	E	184	SER	2.2
1	C	143	GLN	2.2
1	H	105	LEU	2.2
1	H	134	ILE	2.1
1	H	95	LYS	2.1
1	D	143	GLN	2.1
1	C	142	GLY	2.1
1	A	95	LYS	2.0
1	A	101	LYS	2.0
1	F	93	TYR	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.