



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:06 am BST

PDB ID : 5HP5  
Title : Srtucture of human peptidylarginine deiminase type I (PAD1)  
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Deposited on : 2016-01-20  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<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

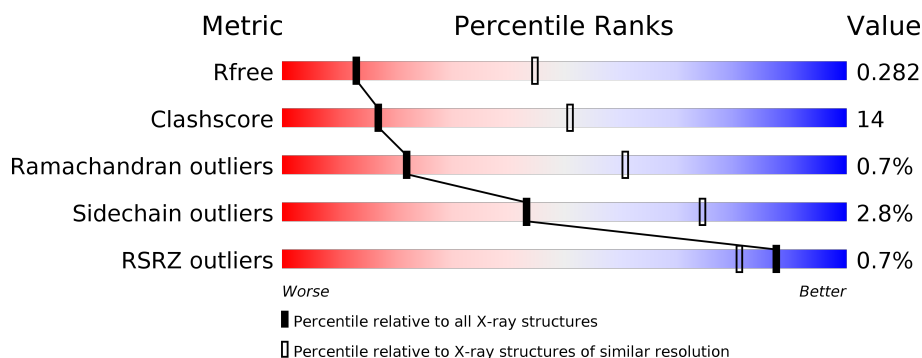
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	684	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>..</div> </div> </div>
1	B	684	<div> <div></div> <div>68%</div> <div>27%</div> <div>...</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10573 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 Protein-arginine deiminase type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	669	Total	C	N	O	S	0	0	0
			5274	3361	903	980	30			
1	B	669	Total	C	N	O	S	0	0	0
			5274	3361	903	980	30			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9ULC6
A	-19	GLY	-	expression tag	UNP Q9ULC6
A	-18	HIS	-	expression tag	UNP Q9ULC6
A	-17	HIS	-	expression tag	UNP Q9ULC6
A	-16	HIS	-	expression tag	UNP Q9ULC6
A	-15	HIS	-	expression tag	UNP Q9ULC6
A	-14	HIS	-	expression tag	UNP Q9ULC6
A	-13	HIS	-	expression tag	UNP Q9ULC6
A	-12	HIS	-	expression tag	UNP Q9ULC6
A	-11	HIS	-	expression tag	UNP Q9ULC6
A	-10	HIS	-	expression tag	UNP Q9ULC6
A	-9	HIS	-	expression tag	UNP Q9ULC6
A	-8	SER	-	expression tag	UNP Q9ULC6
A	-7	SER	-	expression tag	UNP Q9ULC6
A	-6	GLY	-	expression tag	UNP Q9ULC6
A	-5	HIS	-	expression tag	UNP Q9ULC6
A	-4	ILE	-	expression tag	UNP Q9ULC6
A	-3	GLU	-	expression tag	UNP Q9ULC6
A	-2	GLY	-	expression tag	UNP Q9ULC6
A	-1	ARG	-	expression tag	UNP Q9ULC6
A	0	HIS	-	expression tag	UNP Q9ULC6
B	-20	MET	-	expression tag	UNP Q9ULC6
B	-19	GLY	-	expression tag	UNP Q9ULC6
B	-18	HIS	-	expression tag	UNP Q9ULC6
B	-17	HIS	-	expression tag	UNP Q9ULC6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q9ULC6
B	-15	HIS	-	expression tag	UNP Q9ULC6
B	-14	HIS	-	expression tag	UNP Q9ULC6
B	-13	HIS	-	expression tag	UNP Q9ULC6
B	-12	HIS	-	expression tag	UNP Q9ULC6
B	-11	HIS	-	expression tag	UNP Q9ULC6
B	-10	HIS	-	expression tag	UNP Q9ULC6
B	-9	HIS	-	expression tag	UNP Q9ULC6
B	-8	SER	-	expression tag	UNP Q9ULC6
B	-7	SER	-	expression tag	UNP Q9ULC6
B	-6	GLY	-	expression tag	UNP Q9ULC6
B	-5	HIS	-	expression tag	UNP Q9ULC6
B	-4	ILE	-	expression tag	UNP Q9ULC6
B	-3	GLU	-	expression tag	UNP Q9ULC6
B	-2	GLY	-	expression tag	UNP Q9ULC6
B	-1	ARG	-	expression tag	UNP Q9ULC6
B	0	HIS	-	expression tag	UNP Q9ULC6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

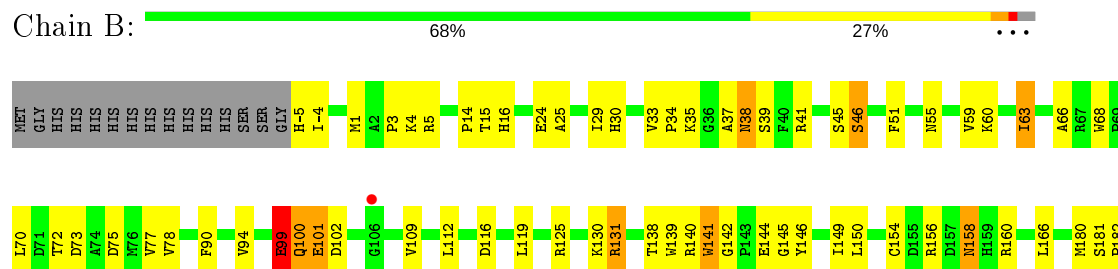
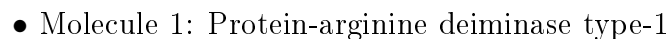
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Ca 4 4	0	0
2	A	4	Total Ca 4 4	0	0

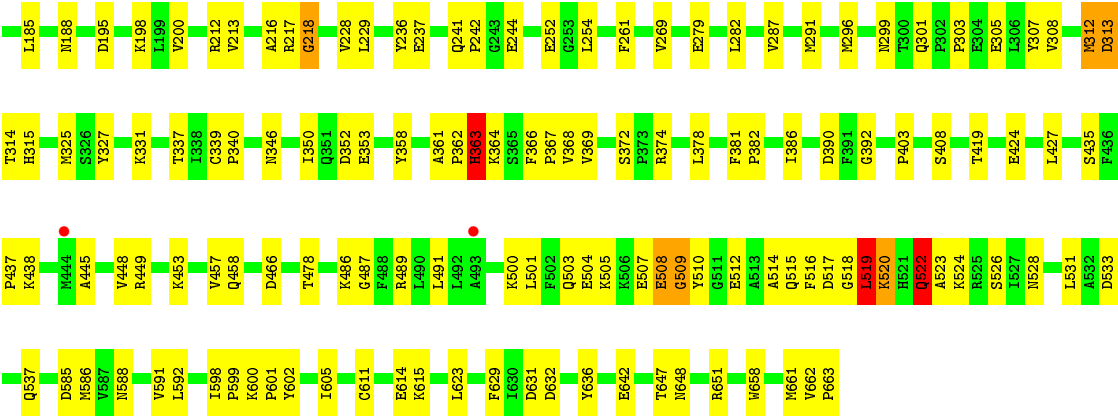
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	9	Total O 9 9	0	0



- Molecule 1: Protein-arginine deiminase type-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.81Å 90.81Å 373.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.73 – 3.20 48.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.73-3.20) 99.9 (48.77-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.213 , 0.278 0.220 , 0.282	Depositor DCC
$R_{free}$ test set	1443 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.2	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 30.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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:  
CA

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	0.33	0/5408	0.65	5/7336 (0.1%)
1	B	0.32	0/5408	0.65	6/7336 (0.1%)
All	All	0.32	0/10816	0.65	11/14672 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	12
All	All	0	23

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	522	GLN	CA-CB-CG	9.52	134.34	113.40
1	B	218	GLY	N-CA-C	-8.46	91.96	113.10
1	A	218	GLY	N-CA-C	-7.55	94.22	113.10
1	B	509	GLY	N-CA-C	7.46	131.74	113.10
1	A	41	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	41	ARG	CG-CD-NE	6.19	124.81	111.80
1	B	142	GLY	N-CA-C	5.86	127.76	113.10
1	B	522	GLN	CB-CA-C	-5.52	99.35	110.40
1	B	519	LEU	CB-CA-C	5.51	120.66	110.20
1	A	525	ARG	CG-CD-NE	-5.35	100.57	111.80
1	A	99	GLU	CA-CB-CG	5.34	125.14	113.40



There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	THR	Peptide
1	A	130	LYS	Peptide
1	A	133	GLN	Peptide
1	A	218	GLY	Peptide
1	A	312	MET	Peptide
1	A	313	ASP	Peptide
1	A	362	PRO	Peptide
1	A	363	HIS	Peptide
1	A	509	GLY	Peptide
1	A	520	LYS	Peptide
1	A	525	ARG	Peptide
1	B	130	LYS	Peptide
1	B	141	TRP	Peptide
1	B	218	GLY	Peptide
1	B	312	MET	Peptide
1	B	313	ASP	Peptide
1	B	314	THR	Peptide
1	B	34	PRO	Peptide
1	B	363	HIS	Peptide
1	B	519	LEU	Peptide
1	B	522	GLN	Peptide
1	B	55	ASN	Peptide
1	B	99	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5274	0	5174	162	0
1	B	5274	0	5174	130	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	8	0	0	2	0
3	B	9	0	0	1	0
All	All	10573	0	10348	292	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 14.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLU:HA	1:B:101:GLU:HG2	1.31	1.10
1:B:101:GLU:HB2	1:B:102:ASP:HA	1.41	1.02
1:A:56:ARG:HH12	1:A:59:VAL:HG22	1.28	0.95
1:A:312:MET:SD	1:A:313:ASP:HA	2.10	0.92
1:A:515:GLN:N	1:A:525:ARG:O	2.09	0.84
1:B:101:GLU:CB	1:B:102:ASP:HA	2.06	0.80
1:A:102:ASP:O	1:A:103:GLN:NE2	2.15	0.80
1:B:363:HIS:O	1:B:363:HIS:ND1	2.15	0.79
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.47	0.79
1:A:100:GLN:NE2	1:A:100:GLN:HA	2.00	0.77
1:A:509:GLY:O	1:A:511:GLY:N	2.17	0.77
1:B:611:CYS:HA	1:B:614:GLU:HG2	1.67	0.76
1:A:123:THR:O	1:A:125:ARG:NE	2.19	0.76
1:A:398:ILE:HD11	1:A:445:ALA:HB2	1.69	0.75
1:A:343:GLU:OE2	1:A:385:ARG:NE	2.22	0.72
1:B:369:VAL:HG21	1:B:386:ILE:HG21	1.72	0.70
1:A:41:ARG:NE	1:A:66:ALA:O	2.19	0.70
1:A:457:VAL:O	1:A:459:ALA:N	2.25	0.69
1:A:27:VAL:HG22	1:A:76:MET:HB3	1.75	0.69
1:A:158:ASN:OD1	1:A:160:ARG:N	2.26	0.68
1:B:427:LEU:HD12	1:B:457:VAL:HG11	1.76	0.68
1:B:522:GLN:HB2	1:B:524:LYS:HE2	1.76	0.68
1:A:41:ARG:NH2	1:A:63:ILE:HG22	2.10	0.67
1:B:500:LYS:NZ	1:B:504:GLU:OE2	2.28	0.67
1:A:101:GLU:HB3	1:A:102:ASP:HA	1.77	0.67
1:B:486:LYS:HB2	1:B:487:GLY:HA2	1.77	0.66
1:A:56:ARG:HG2	1:A:58:ARG:H	1.60	0.66
1:B:138:THR:HG23	1:B:139:TRP:H	1.61	0.66
1:B:350:ILE:HG23	1:B:648:ASN:HB2	1.76	0.66
1:B:602:TYR:OH	1:B:631:ASP:OD2	2.13	0.66
1:A:358:TYR:HA	1:A:367:PRO:HA	1.76	0.65
1:A:552:ASN:OD1	1:A:553:VAL:N	2.30	0.65
1:B:25:ALA:HB3	1:B:78:VAL:HG23	1.79	0.64
1:A:445:ALA:HB3	1:A:448:VAL:HG22	1.80	0.64
1:A:125:ARG:N	1:A:125:ARG:HD3	2.08	0.64
1:B:29:ILE:HD11	1:B:94:VAL:HG11	1.81	0.63
1:A:350:ILE:HG23	1:A:648:ASN:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLY:O	1:A:527:ILE:HB	1.99	0.63
1:B:313:ASP:HB3	1:B:315:HIS:H	1.64	0.63
1:A:531:LEU:HA	1:A:537:GLN:HE22	1.63	0.62
1:B:514:ALA:HA	1:B:526:SER:HA	1.80	0.62
1:B:4:LYS:HD3	1:B:4:LYS:N	2.15	0.62
1:B:519:LEU:HB2	1:B:520:LYS:CB	2.30	0.62
1:A:525:ARG:NH2	1:A:530:MET:HG2	2.16	0.61
1:A:435:SER:HA	1:A:466:ASP:HB2	1.82	0.61
1:A:427:LEU:HD12	1:A:457:VAL:HG11	1.83	0.60
1:A:102:ASP:OD2	1:A:103:GLN:HG2	2.02	0.60
1:A:131:ARG:O	1:A:131:ARG:HG3	2.01	0.59
1:A:213:VAL:HB	1:A:229:LEU:HB2	1.85	0.59
1:B:145:GLY:O	1:B:146:TYR:HD1	1.86	0.59
1:A:56:ARG:NH1	1:A:59:VAL:HG22	2.10	0.58
1:B:366:PHE:HB2	1:B:390:ASP:O	2.03	0.58
1:A:372:SER:O	3:A:801:HOH:O	2.17	0.58
1:A:363:HIS:CD2	1:A:364:LYS:HA	2.38	0.58
1:B:141:TRP:CD1	1:B:661:MET:O	2.56	0.58
1:A:369:VAL:HG21	1:A:386:ILE:HG21	1.86	0.58
1:B:14:PRO:HB3	1:B:109:VAL:HB	1.85	0.58
1:A:361:ALA:HB3	1:A:364:LYS:H	1.69	0.57
1:A:363:HIS:HD2	1:A:364:LYS:HA	1.68	0.57
1:B:512:GLU:OE2	1:B:528:ASN:ND2	2.37	0.57
1:A:604:PRO:HG2	1:A:611:CYS:SG	2.44	0.57
1:B:312:MET:H	1:B:346:ASN:ND2	2.03	0.57
1:A:366:PHE:HB2	1:A:390:ASP:O	2.04	0.57
1:B:90:PHE:HB2	1:B:112:LEU:HB2	1.86	0.57
1:B:37:ALA:HA	1:B:100:GLN:HG3	1.85	0.57
1:A:41:ARG:HD2	1:A:42:VAL:N	2.20	0.56
1:A:529:GLU:HA	1:A:532:ALA:HB3	1.86	0.56
1:A:398:ILE:HG22	1:A:399:PRO:O	2.06	0.56
1:B:368:VAL:HG22	1:B:392:GLY:HA3	1.87	0.56
1:B:435:SER:HA	1:B:466:ASP:HB2	1.88	0.56
1:B:437:PRO:HB2	1:B:438:LYS:HD2	1.88	0.56
1:A:129:VAL:HG11	1:A:184:LEU:HG	1.89	0.55
1:A:326:SER:HA	1:A:336:LEU:HD22	1.89	0.54
1:B:125:ARG:HD3	1:B:149:ILE:HD11	1.90	0.54
1:A:185:LEU:HD13	1:A:269:VAL:HG21	1.89	0.54
1:A:305:GLU:OE2	1:A:337:THR:OG1	2.25	0.54
1:A:368:VAL:HG22	1:A:392:GLY:HA3	1.90	0.54
1:A:303:PRO:HG3	1:A:592:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:THR:OG1	1:A:279:GLU:HA	2.08	0.54
1:A:585:ASP:HB3	1:A:642:GLU:HG3	1.89	0.54
1:A:609:ARG:NH2	1:A:613:GLU:OE1	2.41	0.54
1:B:119:LEU:HD22	1:B:269:VAL:HG23	1.90	0.54
1:B:515:GLN:NE2	1:B:602:TYR:O	2.41	0.54
1:B:503:GLN:O	1:B:507:GLU:HG3	2.08	0.53
1:B:516:PHE:HB3	1:B:519:LEU:HD11	1.89	0.53
1:A:526:SER:HB3	1:A:529:GLU:OE1	2.08	0.53
1:A:29:ILE:HD11	1:A:94:VAL:HG11	1.91	0.53
1:B:372:SER:O	3:B:801:HOH:O	2.19	0.53
1:A:59:VAL:O	1:A:59:VAL:HG23	2.09	0.53
1:B:29:ILE:HG22	1:B:30:HIS:HD2	1.75	0.52
1:A:119:LEU:HD22	1:A:269:VAL:HG23	1.91	0.52
1:B:138:THR:HG23	1:B:139:TRP:N	2.23	0.52
1:B:1:MET:HG3	1:B:4:LYS:NZ	2.25	0.52
1:A:240:ARG:NH2	1:A:245:GLN:HG2	2.24	0.52
1:B:158:ASN:OD1	1:B:160:ARG:N	2.42	0.52
1:A:352:ASP:HB3	1:A:408:SER:HB3	1.92	0.52
1:A:99:GLU:O	1:A:99:GLU:HG2	2.09	0.52
1:A:341:GLN:HE21	1:A:346:ASN:HD22	1.57	0.52
1:A:449:ARG:O	1:A:453:LYS:HG2	2.09	0.52
1:A:153:ASN:O	1:A:166:LEU:HB2	2.10	0.51
1:A:53:VAL:N	1:A:75:ASP:OD2	2.35	0.51
1:B:445:ALA:HB3	1:B:448:VAL:HG22	1.92	0.51
1:B:51:PHE:HB2	1:B:77:VAL:HG23	1.92	0.51
1:A:41:ARG:HH22	1:A:64:GLY:C	2.13	0.51
1:A:517:ASP:OD2	1:A:605:ILE:HG22	2.11	0.51
1:B:140:ARG:H	1:B:146:TYR:HD2	1.57	0.51
1:A:41:ARG:HD2	1:A:42:VAL:H	1.74	0.51
1:B:301:GLN:HB2	1:B:651:ARG:HD3	1.92	0.51
1:B:327:TYR:O	1:B:331:LYS:HG2	2.11	0.51
1:B:228:VAL:HB	1:B:236:TYR:CG	2.46	0.51
1:B:75:ASP:N	1:B:75:ASP:OD1	2.42	0.51
1:A:308:VAL:O	1:A:338:ILE:HA	2.10	0.51
1:B:279:GLU:OE1	1:B:279:GLU:N	2.44	0.51
1:A:140:ARG:H	1:A:146:TYR:CB	2.24	0.50
1:A:525:ARG:CZ	1:A:530:MET:HG2	2.42	0.50
1:B:457:VAL:HG12	1:B:458:GLN:HG3	1.93	0.50
1:B:308:VAL:HG23	1:B:647:THR:HG22	1.93	0.50
1:A:589:MET:O	1:A:644:HIS:HB2	2.11	0.50
1:B:139:TRP:HA	1:B:146:TYR:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:GLU:HG3	1:B:615:LYS:N	2.26	0.50
1:A:101:GLU:HB3	1:A:102:ASP:CA	2.41	0.50
1:A:90:PHE:HB2	1:A:112:LEU:HB2	1.93	0.50
1:A:5:ARG:NH1	1:A:18:VAL:O	2.44	0.50
1:B:33:VAL:HG11	1:B:70:LEU:HD21	1.93	0.50
1:A:513:ALA:O	1:A:527:ILE:HG13	2.12	0.50
1:B:116:ASP:HB3	1:B:188:ASN:HB3	1.93	0.50
1:B:305:GLU:OE2	1:B:337:THR:OG1	2.28	0.49
1:B:3:PRO:C	1:B:4:LYS:HD3	2.32	0.49
1:B:531:LEU:O	1:B:537:GLN:NE2	2.45	0.49
1:B:101:GLU:HB2	1:B:102:ASP:CA	2.27	0.49
1:A:41:ARG:NH2	1:A:64:GLY:O	2.43	0.49
1:B:185:LEU:HD13	1:B:269:VAL:HG21	1.93	0.49
1:B:449:ARG:O	1:B:453:LYS:HG2	2.13	0.49
1:B:505:LYS:HA	1:B:508:GLU:HG2	1.93	0.49
1:B:501:LEU:HD13	1:B:615:LYS:HD3	1.94	0.49
1:A:212:ARG:HG3	1:A:254:LEU:HD21	1.94	0.49
1:A:125:ARG:NH2	1:A:146:TYR:C	2.66	0.49
1:A:72:THR:HG22	1:A:73:ASP:H	1.78	0.49
1:B:353:GLU:HG2	1:B:378:LEU:HB3	1.95	0.49
1:B:303:PRO:HG3	1:B:592:LEU:HB3	1.95	0.49
1:B:156:ARG:HB3	1:B:158:ASN:O	2.13	0.49
1:B:99:GLU:HA	1:B:101:GLU:H	1.78	0.49
1:A:116:ASP:HB3	1:A:188:ASN:HB3	1.93	0.49
1:A:512:GLU:OE2	1:A:528:ASN:ND2	2.44	0.49
1:A:602:TYR:OH	1:A:631:ASP:OD2	2.30	0.48
1:A:657:LYS:HG2	1:A:659:TRP:CZ2	2.47	0.48
1:B:139:TRP:HA	1:B:146:TYR:CD2	2.48	0.48
1:B:586:MET:SD	1:B:601:PRO:HG3	2.53	0.48
1:A:586:MET:SD	1:A:601:PRO:HG3	2.53	0.48
1:A:596:LEU:HD11	1:A:625:LEU:HD13	1.94	0.48
1:B:489:ARG:HE	1:B:623:LEU:HD21	1.77	0.48
1:A:51:PHE:HB2	1:A:77:VAL:HG23	1.95	0.48
1:A:525:ARG:NH1	1:A:526:SER:O	2.47	0.48
1:A:151:LEU:HG	1:A:361:ALA:HB2	1.95	0.48
1:A:87:LEU:HD12	1:A:113:THR:HG21	1.94	0.48
1:A:160:ARG:NH2	1:A:172:MET:HG3	2.28	0.48
1:B:307:TYR:HB3	1:B:350:ILE:HD13	1.96	0.48
1:B:141:TRP:HZ2	1:B:658:TRP:O	1.97	0.48
1:B:509:GLY:CA	1:B:510:TYR:HB2	2.44	0.47
1:A:166:LEU:HD11	1:A:254:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASP:OD2	1:B:605:ILE:HG22	2.14	0.47
1:B:138:THR:CG2	1:B:139:TRP:H	2.25	0.47
1:B:24:GLU:OE2	1:B:60:LYS:NZ	2.31	0.47
1:B:131:ARG:O	1:B:131:ARG:HG2	2.14	0.47
1:A:53:VAL:H	1:A:75:ASP:CG	2.17	0.47
1:A:348:ARG:HD2	1:A:639:LEU:HD12	1.95	0.47
1:A:512:GLU:OE1	1:A:526:SER:CB	2.63	0.47
1:A:525:ARG:HD2	1:A:526:SER:N	2.29	0.47
1:B:141:TRP:CD1	1:B:662:VAL:HA	2.50	0.47
1:B:438:LYS:HD2	1:B:438:LYS:N	2.30	0.47
1:B:41:ARG:HG3	1:B:66:ALA:O	2.15	0.47
1:B:585:ASP:HB3	1:B:642:GLU:HG3	1.96	0.47
1:A:484:ASP:OD1	1:A:489:ARG:NH2	2.48	0.46
1:B:588:ASN:OD1	1:B:642:GLU:HB2	2.15	0.46
1:A:98:GLY:HA3	1:A:100:GLN:HB3	1.97	0.46
1:A:327:TYR:O	1:A:331:LYS:HG2	2.16	0.46
1:B:213:VAL:HB	1:B:229:LEU:HB2	1.96	0.46
1:A:264:LEU:HD23	1:A:290:ARG:HG2	1.98	0.46
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.23	0.46
1:A:512:GLU:OE1	1:A:526:SER:HB2	2.15	0.46
1:A:101:GLU:HB3	1:A:102:ASP:O	2.16	0.46
1:A:515:GLN:NE2	1:A:602:TYR:O	2.49	0.46
1:B:374:ARG:HA	1:B:403:PRO:HG2	1.97	0.46
1:B:38:ASN:OD1	1:B:39:SER:OG	2.33	0.46
1:B:180:MET:HG2	1:B:252:GLU:HB3	1.97	0.46
1:B:29:ILE:HG22	1:B:30:HIS:CD2	2.51	0.46
1:B:358:TYR:HA	1:B:367:PRO:HA	1.98	0.45
1:A:312:MET:CE	1:A:317:SER:HA	2.46	0.45
1:A:609:ARG:HG3	1:A:614:GLU:OE2	2.17	0.45
1:B:-5:HIS:CE1	1:B:-4:ILE:HD12	2.50	0.45
1:A:156:ARG:O	1:A:389:PRO:HA	2.17	0.45
1:B:158:ASN:OD1	1:B:160:ARG:HB2	2.17	0.45
1:A:632:ASP:HB2	1:A:636:TYR:HB2	1.98	0.45
1:B:72:THR:HG22	1:B:73:ASP:H	1.82	0.45
1:A:181:SER:HA	1:A:182:PRO:HD3	1.80	0.45
1:A:307:TYR:HB3	1:A:350:ILE:HD13	1.99	0.45
1:A:613:GLU:O	1:A:617:GLN:HG3	2.17	0.45
1:A:591:VAL:O	1:A:651:ARG:NH2	2.41	0.45
1:A:455:GLN:C	1:A:457:VAL:H	2.19	0.44
1:B:15:THR:HG22	1:B:16:HIS:H	1.81	0.44
1:B:518:GLY:HA3	1:B:602:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:NH1	1:A:147:GLY:O	2.46	0.44
1:A:419:THR:HG22	1:A:424:GLU:HB2	1.99	0.44
1:B:158:ASN:C	1:B:158:ASN:OD1	2.55	0.44
1:B:591:VAL:O	1:B:651:ARG:NH2	2.45	0.44
1:B:141:TRP:NE1	1:B:661:MET:O	2.50	0.44
1:A:140:ARG:H	1:A:146:TYR:HB3	1.81	0.44
1:A:361:ALA:HB1	1:A:362:PRO:HD2	1.99	0.44
1:A:38:ASN:OD1	1:A:39:SER:N	2.50	0.44
1:B:296:MET:H	1:B:458:GLN:HE22	1.66	0.44
1:A:419:THR:HA	1:A:424:GLU:HA	1.98	0.44
1:B:533:ASP:O	1:B:537:GLN:HG3	2.17	0.44
1:B:632:ASP:HB2	1:B:636:TYR:HB2	1.99	0.44
1:A:156:ARG:HB3	1:A:158:ASN:O	2.18	0.44
1:A:312:MET:HE2	1:A:317:SER:HA	2.00	0.44
1:B:241:GLN:HB3	1:B:242:PRO:HD2	2.00	0.44
1:B:478:THR:HG22	1:B:491:LEU:HB2	1.99	0.44
1:A:525:ARG:HD2	1:A:526:SER:H	1.83	0.43
1:A:630:ILE:HB	1:A:643:ILE:HD11	1.99	0.43
1:B:261:PHE:HE2	1:B:291:MET:HG3	1.83	0.43
1:B:299:ASN:HA	1:B:651:ARG:CZ	2.48	0.43
1:B:661:MET:HG3	1:B:663:PRO:HD3	2.00	0.43
1:B:308:VAL:HG21	1:B:325:MET:HG2	2.00	0.43
1:B:519:LEU:HD13	1:B:520:LYS:CB	2.48	0.43
1:A:140:ARG:O	1:A:146:TYR:HB3	2.18	0.43
1:A:514:ALA:O	1:A:604:PRO:HA	2.18	0.43
1:B:381:PHE:HB3	1:B:382:PRO:HD3	2.00	0.43
1:A:158:ASN:ND2	1:A:172:MET:HG2	2.33	0.43
1:A:25:ALA:HB3	1:A:78:VAL:CG2	2.49	0.43
1:B:45:SER:HA	1:B:46:SER:HA	1.54	0.43
1:A:531:LEU:HA	1:A:537:GLN:NE2	2.31	0.43
1:B:166:LEU:HD11	1:B:254:LEU:O	2.19	0.43
1:B:352:ASP:HB3	1:B:408:SER:HB3	2.00	0.43
1:B:524:LYS:HD3	1:B:524:LYS:N	2.33	0.43
1:A:353:GLU:HG2	1:A:378:LEU:HB3	1.99	0.43
1:A:138:THR:O	1:A:147:GLY:HA3	2.18	0.43
1:A:180:MET:HG2	1:A:252:GLU:HB3	1.99	0.43
1:A:442:ARG:HE	1:A:449:ARG:CZ	2.31	0.43
1:A:366:PHE:HA	1:A:367:PRO:HD3	1.84	0.43
1:A:519:LEU:HG	1:A:520:LYS:H	1.84	0.43
1:A:131:ARG:O	1:A:131:ARG:CG	2.65	0.43
1:A:516:PHE:HA	1:A:602:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:NH2	1:B:244:GLU:OE1	2.51	0.43
1:A:381:PHE:HB3	1:A:382:PRO:HD3	2.00	0.42
1:A:39:SER:HA	1:A:70:LEU:HB2	2.00	0.42
1:B:598:ILE:HA	1:B:599:PRO:HD2	1.93	0.42
1:A:99:GLU:N	1:A:100:GLN:HB3	2.34	0.42
1:A:154:CYS:O	1:A:392:GLY:HA2	2.19	0.42
1:A:309:CYS:HB2	1:A:344:ASN:HD22	1.85	0.42
1:A:41:ARG:HD3	1:A:41:ARG:HA	1.37	0.42
1:A:158:ASN:OD1	1:A:158:ASN:C	2.57	0.42
1:A:290:ARG:NH1	3:A:803:HOH:O	2.37	0.42
1:A:341:GLN:HE21	1:A:346:ASN:ND2	2.18	0.42
1:A:430:ILE:O	1:A:460:PRO:HA	2.20	0.42
1:A:502:PHE:HE2	1:A:571:LEU:HD11	1.84	0.42
1:A:156:ARG:C	1:A:158:ASN:H	2.21	0.42
1:A:478:THR:HG22	1:A:491:LEU:HB2	2.00	0.42
1:B:5:ARG:HD3	1:B:282:LEU:HD22	2.02	0.42
1:A:14:PRO:HB3	1:A:109:VAL:HB	2.02	0.42
1:A:482:THR:HB	1:A:484:ASP:O	2.20	0.42
1:A:599:PRO:HB3	1:A:632:ASP:OD2	2.19	0.42
1:A:301:GLN:HB2	1:A:651:ARG:HD3	2.02	0.42
1:A:184:LEU:HA	1:A:184:LEU:HD23	1.92	0.42
1:B:312:MET:HG3	1:B:313:ASP:OD1	2.20	0.41
1:B:419:THR:HA	1:B:424:GLU:HA	2.02	0.41
1:B:181:SER:HA	1:B:182:PRO:HD3	1.81	0.41
1:A:261:PHE:HE2	1:A:291:MET:HG3	1.84	0.41
1:A:45:SER:HA	1:A:46:SER:HA	1.73	0.41
1:A:476:PHE:C	1:A:587:VAL:HG11	2.41	0.41
1:B:361:ALA:HB1	1:B:362:PRO:HD2	2.01	0.41
1:A:489:ARG:HE	1:A:623:LEU:HD21	1.86	0.41
1:A:299:ASN:HA	1:A:651:ARG:CZ	2.50	0.41
1:B:523:ALA:C	1:B:524:LYS:HD3	2.41	0.41
1:B:150:LEU:HD11	1:B:252:GLU:HA	2.01	0.41
1:A:588:ASN:OD1	1:A:642:GLU:HB2	2.21	0.41
1:B:149:ILE:HD12	1:B:362:PRO:HD3	2.03	0.41
1:B:364:LYS:HA	1:B:364:LYS:HD2	1.72	0.41
1:B:29:ILE:HD11	1:B:94:VAL:HG21	2.02	0.41
1:A:449:ARG:HB3	1:A:453:LYS:HE2	2.03	0.41
1:A:328:LEU:O	1:A:331:LYS:HG3	2.20	0.41
1:B:600:LYS:HG3	1:B:629:PHE:HB3	2.03	0.41
1:A:101:GLU:CB	1:A:102:ASP:HA	2.48	0.41
1:A:274:PRO:C	1:A:276:THR:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:HG3	1:B:254:LEU:HD21	2.02	0.41
1:B:216:ALA:O	1:B:217:ARG:HD2	2.20	0.40
1:B:63:ILE:HG12	1:B:68:TRP:CZ3	2.57	0.40
1:B:195:ASP:O	1:B:198:LYS:NZ	2.45	0.40
1:B:599:PRO:HB3	1:B:632:ASP:OD2	2.21	0.40
1:B:339:CYS:HA	1:B:340:PRO:HD2	1.96	0.40
1:A:311:VAL:HG12	1:A:346:ASN:HA	2.03	0.40
1:A:589:MET:HB2	1:A:597:GLY:O	2.22	0.40
1:B:154:CYS:O	1:B:392:GLY:HA2	2.20	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:B:99:GLU:OE2	1:B:212:ARG:NH1[5_664]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	667/684 (98%)	630 (94%)	33 (5%)	4 (1%)	25	64
1	B	667/684 (98%)	628 (94%)	34 (5%)	5 (1%)	22	61
All	All	1334/1368 (98%)	1258 (94%)	67 (5%)	9 (1%)	22	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	GLN
1	A	510	TYR
1	A	457	VAL
1	B	100	GLN

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Mol	Chain	Res	Type
1	B	520	LYS
1	B	131	ARG
1	B	35	LYS
1	A	59	VAL
1	B	59	VAL

### 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	581/601 (97%)	562 (97%)	19 (3%)	38	71
1	B	581/601 (97%)	568 (98%)	13 (2%)	52	79
All	All	1162/1202 (97%)	1130 (97%)	32 (3%)	43	74

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	43	SER
1	A	56	ARG
1	A	99	GLU
1	A	100	GLN
1	A	128	LYS
1	A	129	VAL
1	A	158	ASN
1	A	160	ARG
1	A	169	SER
1	A	272	VAL
1	A	279	GLU
1	A	346	ASN
1	A	438	LYS
1	A	507	GLU
1	A	522	GLN
1	A	524	LYS
1	A	525	ARG

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Mol	Chain	Res	Type
1	A	526	SER
1	B	38	ASN
1	B	46	SER
1	B	63	ILE
1	B	99	GLU
1	B	101	GLU
1	B	144	GLU
1	B	158	ASN
1	B	200	VAL
1	B	237	GLU
1	B	287	VAL
1	B	363	HIS
1	B	508	GLU
1	B	519	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	103	GLN
1	A	341	GLN
1	A	363	HIS
1	B	30	HIS
1	B	341	GLN
1	B	346	ASN
1	B	458	GLN
1	B	528	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	669/684 (97%)	0.12	6 (0%)	84 75	53, 78, 115, 134	0
1	B	669/684 (97%)	0.09	3 (0%)	92 89	53, 79, 113, 140	0
All	All	1338/1368 (97%)	0.11	9 (0%)	87 81	53, 78, 115, 140	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	444	MET	5.0
1	A	444	MET	4.9
1	A	518	GLY	4.6
1	B	106	GLY	2.7
1	A	479	PHE	2.6
1	B	493	ALA	2.5
1	A	74	ALA	2.4
1	A	519	LEU	2.2
1	A	265	VAL	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( $\text{\AA}^2$ )	Q<0.9
2	CA	A	702	1/1	0.92	0.18	64,64,64,64	0
2	CA	B	702	1/1	0.95	0.15	60,60,60,60	0
2	CA	A	701	1/1	0.97	0.18	64,64,64,64	0
2	CA	B	704	1/1	0.98	0.11	82,82,82,82	0
2	CA	B	701	1/1	0.98	0.22	68,68,68,68	0
2	CA	A	704	1/1	0.98	0.12	80,80,80,80	0
2	CA	A	703	1/1	0.99	0.14	65,65,65,65	0
2	CA	B	703	1/1	1.00	0.17	59,59,59,59	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.