



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:47 AM GMT

PDB ID : 2DRW  
Title : The crystal structure of D-amino acid amidase from Ochrobactrum anthropi SV3  
Authors : Okazaki, S.; Suzuki, A.; Komeda, H.; Asano, Y.; Yamane, T.  
Deposited on : 2006-06-15  
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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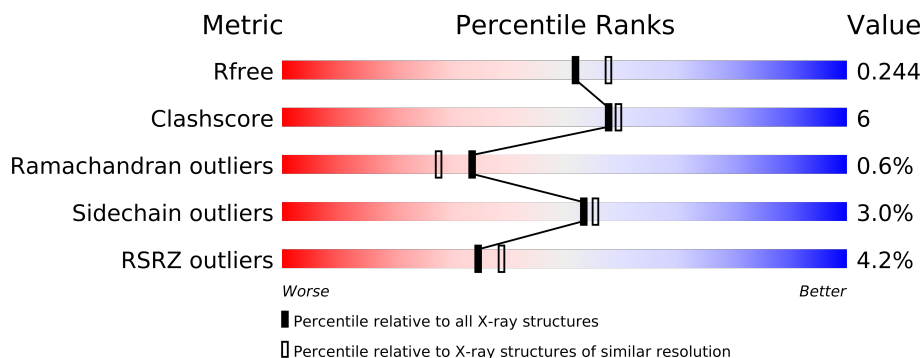
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	BA	A	3009	-	X
2	BA	B	3010	-	X
2	BA	F	3008	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18459 atoms, of which 0 are hydrogen and 0 are deuterium.

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 D-Amino acid amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2811	1775	486	534	16			
1	B	362	Total	C	N	O	S	0	2	0
			2827	1784	488	538	17			
1	C	358	Total	C	N	O	S	0	0	0
			2787	1762	482	527	16			
1	D	350	Total	C	N	O	S	0	0	0
			2718	1720	471	511	16			
1	E	345	Total	C	N	O	S	0	0	0
			2685	1699	466	504	16			
1	F	327	Total	C	N	O	S	0	0	0
			2552	1622	439	475	16			

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	5	Total	Ba	0	0
			5	5		
2	E	3	Total	Ba	0	0
			3	3		
2	B	2	Total	Ba	0	0
			2	2		
2	C	3	Total	Ba	0	0
			3	3		
2	A	4	Total	Ba	0	0
			4	4		
2	F	6	Total	Ba	0	0
			6	6		

- Molecule 3 is water.

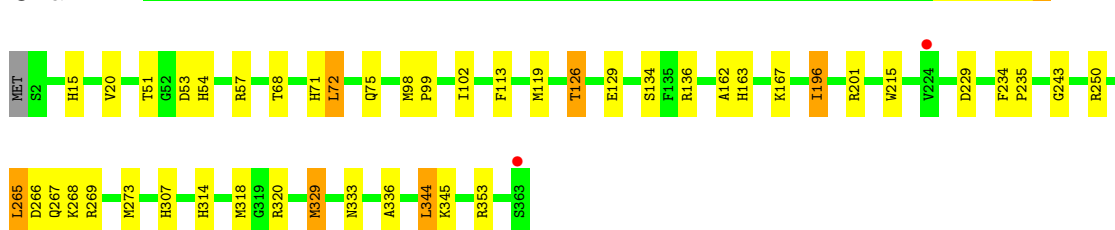
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	358	Total 358	O 358	0	0
3	B	438	Total 438	O 438	0	0
3	C	393	Total 393	O 393	0	0
3	D	385	Total 385	O 385	0	0
3	E	258	Total 258	O 258	0	0
3	F	224	Total 224	O 224	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

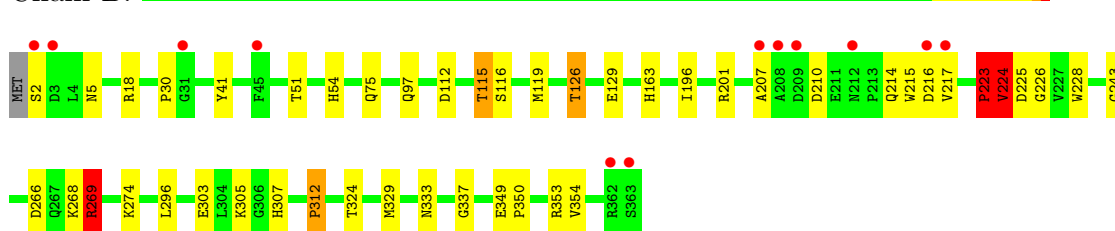
- Molecule 1: D-Amino acid amidase

Chain A:



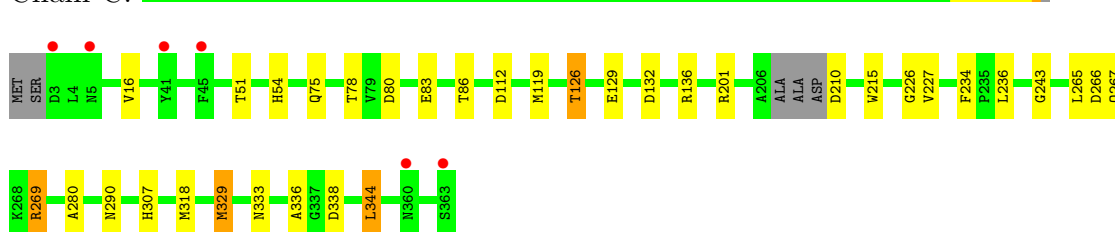
- Molecule 1: D-Amino acid amidase

Chain B:



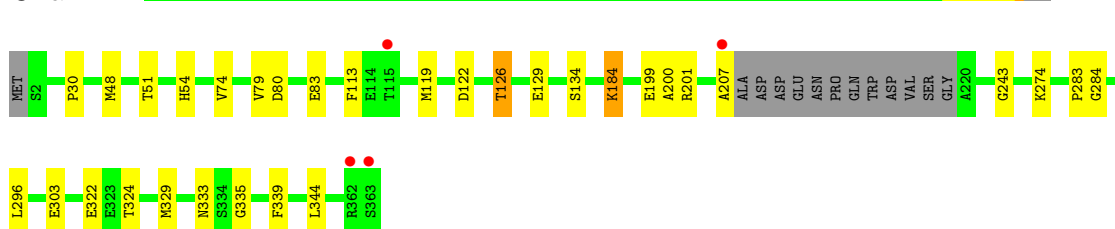
- Molecule 1: D-Amino acid amidase

Chain C:

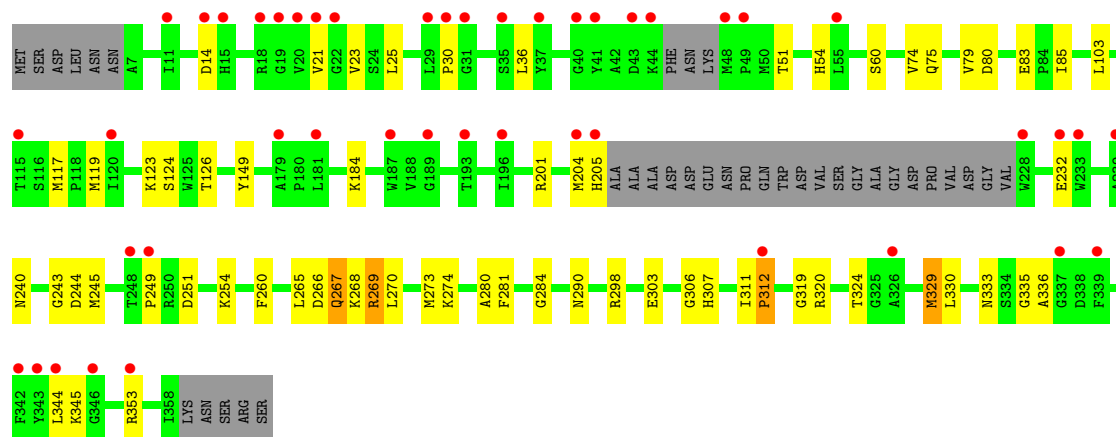


- Molecule 1: D-Amino acid amidase

Chain D:



- Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.20Å 123.22Å 115.71Å 90.00° 104.36° 90.00°	Depositor
Resolution (Å)	47.57 – 2.10 47.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.57-2.10) 99.9 (47.55-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.182 , 0.243 0.183 , 0.244	Depositor DCC
$R_{free}$ test set	6124 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 122003 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.50	0/2883	0.62	0/3910
1	B	0.54	0/2899	0.68	3/3931 (0.1%)
1	C	0.50	0/2858	0.61	0/3874
1	D	0.52	0/2786	0.61	0/3774
1	E	0.45	0/2751	0.56	0/3724
1	F	0.49	0/2617	0.57	0/3544
All	All	0.50	0/16794	0.61	3/22757 (0.0%)

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	B	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	VAL	N-CA-C	6.71	129.11	111.00
1	B	269	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	226	GLY	N-CA-C	-5.39	99.64	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	223	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	224	VAL	Peptide
1	B	225	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2811	0	2710	44	0
1	B	2827	0	2722	33	0
1	C	2787	0	2691	28	0
1	D	2718	0	2639	18	0
1	E	2685	0	2613	32	0
1	F	2552	0	2482	54	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
2	E	3	0	0	0	0
2	F	6	0	0	0	0
3	A	358	0	0	8	0
3	B	438	0	0	9	2
3	C	393	0	0	4	1
3	D	385	0	0	4	1
3	E	258	0	0	1	0
3	F	224	0	0	9	0
All	All	18459	0	15857	201	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (201) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:265:LEU:HD12	1:F:273:MET:CE	1.77	1.14
1:F:265:LEU:CD1	1:F:273:MET:CE	2.29	1.10
1:A:102:ILE:HG21	3:A:3366:HOH:O	1.53	1.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:TYR:HE1	3:B:3436:HOH:O	1.47	0.97
1:A:353:ARG:NH1	3:A:3375:HOH:O	1.96	0.95
1:F:265:LEU:CD1	1:F:273:MET:HE1	1.98	0.93
1:C:267:GLN:HE22	1:E:284:GLY:H	1.18	0.92
1:F:51:THR:H	1:F:54:HIS:HD2	1.19	0.90
1:F:320:ARG:HD3	3:F:3242:HOH:O	1.73	0.89
1:F:265:LEU:HD12	1:F:273:MET:HE1	1.55	0.87
1:A:51:THR:H	1:A:54:HIS:HD2	1.23	0.87
1:B:126:THR:HG21	3:B:3123:HOH:O	1.79	0.81
1:C:51:THR:H	1:C:54:HIS:HD2	1.27	0.80
1:F:298:ARG:HG2	1:F:303:GLU:HG2	1.64	0.80
1:F:265:LEU:HD12	1:F:273:MET:HE3	1.63	0.80
1:A:234:PHE:HB3	3:A:3038:HOH:O	1.82	0.80
1:D:51:THR:H	1:D:54:HIS:HD2	1.27	0.80
1:F:265:LEU:HD11	1:F:273:MET:CE	2.12	0.79
1:A:75:GLN:NE2	1:A:266:ASP:H	1.80	0.79
1:A:72:LEU:HD13	1:A:265:LEU:HD12	1.65	0.78
1:B:51:THR:H	1:B:54:HIS:HD2	1.30	0.78
1:F:265:LEU:CD1	1:F:273:MET:HE2	2.13	0.77
1:E:51:THR:H	1:E:54:HIS:HD2	1.31	0.77
1:B:41:TYR:CE1	3:B:3436:HOH:O	2.25	0.76
1:B:126:THR:HG22	1:B:129:GLU:H	1.52	0.75
1:A:75:GLN:HE22	1:A:266:ASP:H	1.32	0.75
1:C:210:ASP:HA	1:C:338:ASP:HB2	1.68	0.74
1:F:204:MET:HA	1:F:205:HIS:HB2	1.67	0.74
1:E:75:GLN:NE2	1:E:266:ASP:H	1.85	0.74
1:A:126:THR:HG22	1:A:129:GLU:H	1.51	0.74
1:F:75:GLN:HG3	1:F:269:ARG:HD3	1.70	0.73
1:F:265:LEU:HD11	1:F:273:MET:HE1	1.70	0.73
1:C:267:GLN:NE2	1:E:284:GLY:H	1.87	0.72
1:F:51:THR:H	1:F:54:HIS:CD2	2.04	0.72
1:A:196:ILE:HD12	1:A:196:ILE:H	1.54	0.72
1:A:57:ARG:H	1:A:314:HIS:HD2	1.37	0.72
1:A:99:PRO:O	1:A:102:ILE:HG13	1.89	0.72
1:B:75:GLN:HB3	1:B:269:ARG:HD3	1.72	0.71
1:A:98:MET:HB3	1:A:102:ILE:HD11	1.73	0.71
1:F:244:ASP:OD2	3:F:3238:HOH:O	2.09	0.69
1:A:71:HIS:HD2	1:A:273:MET:HE3	1.57	0.69
1:A:72:LEU:HD13	1:A:265:LEU:CD1	2.22	0.69
1:F:75:GLN:NE2	1:F:266:ASP:H	1.90	0.69
1:E:75:GLN:HE22	1:E:265:LEU:HA	1.56	0.69
1:C:75:GLN:NE2	1:C:266:ASP:H	1.92	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:353:ARG:N	1:E:353:ARG:HD2	2.07	0.68
1:A:268:LYS:HD3	1:F:281:PHE:CD2	2.29	0.67
1:F:245:MET:HB3	3:F:3222:HOH:O	1.95	0.67
1:B:119[A]:MET:HE3	1:B:312:PRO:HG3	1.76	0.67
1:E:46:ASN:N	1:E:47:LYS:HA	2.09	0.67
1:C:75:GLN:HE22	1:C:265:LEU:HA	1.59	0.66
1:E:6:ASN:HB3	3:E:3132:HOH:O	1.95	0.66
1:C:16:VAL:HB	3:C:3381:HOH:O	1.94	0.65
1:D:126:THR:HG22	1:D:129:GLU:H	1.62	0.65
1:E:75:GLN:HE22	1:E:266:ASP:H	1.43	0.64
1:B:30:PRO:HG3	1:B:324:THR:O	1.97	0.64
1:C:267:GLN:HE22	1:E:284:GLY:N	1.92	0.63
1:F:14:ASP:HB2	1:F:353:ARG:HH12	1.63	0.63
1:A:71:HIS:CD2	1:A:273:MET:HE3	2.33	0.62
1:B:266:ASP:OD1	1:B:269:ARG:HD2	1.99	0.62
1:C:269:ARG:NH2	3:C:3189:HOH:O	2.27	0.61
1:C:132:ASP:O	1:C:136:ARG:HG2	2.02	0.60
1:D:207:ALA:HA	3:D:3310:HOH:O	2.03	0.59
1:F:336:ALA:HB3	1:F:344:LEU:HG	1.84	0.58
1:B:163:HIS:HD2	3:B:3129:HOH:O	1.85	0.58
1:C:336:ALA:H	1:C:344:LEU:HD13	1.68	0.58
1:A:72:LEU:CD1	1:A:265:LEU:HD12	2.34	0.58
1:A:71:HIS:HD2	1:A:273:MET:CE	2.15	0.58
1:F:280:ALA:HB2	1:F:290:ASN:OD1	2.03	0.58
1:B:296:LEU:HG	1:B:305:LYS:HE3	1.84	0.57
1:B:51:THR:H	1:B:54:HIS:CD2	2.18	0.57
1:A:336:ALA:H	1:A:344:LEU:HD13	1.69	0.57
1:F:284:GLY:O	1:F:345:LYS:HG3	2.05	0.57
1:C:75:GLN:HG2	1:C:269:ARG:HD3	1.88	0.56
1:B:274:LYS:O	1:B:305:LYS:HE2	2.05	0.56
1:C:75:GLN:HE22	1:C:266:ASP:H	1.53	0.56
1:E:24:SER:HB2	1:E:50:MET:HE2	1.86	0.56
1:B:126:THR:HG23	3:B:3046:HOH:O	2.05	0.56
1:C:126:THR:HG22	1:C:129:GLU:H	1.71	0.56
1:A:75:GLN:HE22	1:A:266:ASP:N	2.04	0.55
1:E:316:SER:HB3	1:E:331:ILE:HG23	1.89	0.55
1:B:119[A]:MET:CE	1:B:312:PRO:HG3	2.36	0.55
1:F:75:GLN:HE22	1:F:265:LEU:HA	1.72	0.54
1:E:46:ASN:O	1:E:46:ASN:CG	2.45	0.54
1:B:5:ASN:HB3	3:B:3421:HOH:O	2.06	0.54
1:D:30:PRO:HG2	1:D:324:THR:O	2.08	0.54
1:E:51:THR:H	1:E:54:HIS:CD2	2.19	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:119:MET:HG3	1:A:215:TRP:HB3	1.89	0.54
1:E:195:PRO:HB2	1:E:198:ARG:HG3	1.90	0.54
1:B:201:ARG:O	1:B:333:ASN:HB2	2.09	0.53
1:D:80:ASP:O	1:D:83:GLU:HG2	2.08	0.53
1:E:265:LEU:HG	1:E:269:ARG:HB3	1.89	0.53
1:B:18:ARG:NH1	1:B:349:GLU:OE1	2.42	0.53
1:A:57:ARG:H	1:A:314:HIS:CD2	2.24	0.52
1:A:75:GLN:HE22	1:A:265:LEU:HA	1.74	0.52
1:B:223:PRO:HD3	1:B:228:TRP:CZ2	2.44	0.52
1:D:51:THR:H	1:D:54:HIS:CD2	2.19	0.51
1:B:349:GLU:HB3	1:B:353:ARG:NH1	2.24	0.51
1:C:201:ARG:O	1:C:333:ASN:HB2	2.10	0.51
1:A:163:HIS:HE1	3:A:3293:HOH:O	1.92	0.51
1:A:53:ASP:OD1	1:A:250:ARG:NH2	2.34	0.51
1:F:265:LEU:HD11	1:F:273:MET:HE2	1.84	0.50
1:A:51:THR:H	1:A:54:HIS:CD2	2.15	0.50
1:A:267:GLN:NE2	1:F:284:GLY:H	2.10	0.50
1:B:350:PRO:O	1:B:354:VAL:HG23	2.12	0.50
1:E:195:PRO:CB	1:E:198:ARG:HG3	2.42	0.49
1:F:123:LYS:HG3	3:F:3067:HOH:O	2.11	0.49
1:E:136:ARG:HG2	1:E:137:HIS:CE1	2.47	0.49
1:F:269:ARG:N	1:F:269:ARG:HD2	2.26	0.49
1:B:115:THR:HG22	3:B:3199:HOH:O	2.12	0.49
1:C:119:MET:HG3	1:C:215:TRP:HB3	1.95	0.49
1:F:267:GLN:NE2	3:F:3171:HOH:O	2.44	0.49
1:B:214:GLN:HG2	1:B:337:GLY:O	2.13	0.49
1:F:240:ASN:HA	3:F:3238:HOH:O	2.12	0.48
1:F:251:ASP:O	1:F:254:LYS:HB2	2.14	0.48
1:D:274:LYS:HD2	1:D:322:GLU:OE2	2.13	0.48
1:A:267:GLN:HE22	1:F:284:GLY:N	2.12	0.48
1:A:163:HIS:CE1	3:A:3293:HOH:O	2.67	0.48
1:E:318:MET:HB3	1:E:329:MET:SD	2.54	0.48
1:E:46:ASN:N	1:E:47:LYS:CA	2.77	0.47
1:D:339:PHE:HA	1:D:344:LEU:HD23	1.94	0.47
1:A:265:LEU:HG	1:A:269:ARG:HB3	1.96	0.47
1:F:306:GLY:HA3	1:F:319:GLY:HA2	1.96	0.47
1:D:113:PHE:HB3	1:D:134:SER:OG	2.14	0.47
1:E:75:GLN:HE22	1:E:266:ASP:N	2.10	0.47
1:C:318:MET:HB3	1:C:329:MET:SD	2.54	0.47
1:F:60:SER:HB3	1:F:149:TYR:OH	2.15	0.47
1:A:126:THR:HG23	3:A:3132:HOH:O	2.15	0.47
1:C:75:GLN:HE22	1:C:265:LEU:CA	2.28	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:266:ASP:OD1	1:C:269:ARG:HD2	2.14	0.46
1:E:201:ARG:O	1:E:333:ASN:HB2	2.15	0.46
1:A:201:ARG:O	1:A:333:ASN:HB2	2.16	0.46
1:F:85:ILE:HD13	1:F:103:LEU:HD21	1.98	0.45
1:A:196:ILE:CD1	1:A:196:ILE:H	2.18	0.45
1:F:270:LEU:O	1:F:274:LYS:HG2	2.16	0.45
1:D:335:GLY:HA3	3:D:3284:HOH:O	2.16	0.45
1:F:205:HIS:HB2	1:F:335:GLY:O	2.16	0.45
1:F:303:GLU:HB2	3:F:3233:HOH:O	2.15	0.45
1:B:296:LEU:CG	1:B:305:LYS:HE3	2.47	0.45
1:C:234:PHE:HB3	3:C:3188:HOH:O	2.16	0.45
1:D:296:LEU:HD11	1:D:303:GLU:OE1	2.17	0.45
1:B:119[B]:MET:HG3	1:B:215:TRP:CD1	2.52	0.45
1:E:201:ARG:HD3	1:E:229:ASP:OD2	2.17	0.45
1:E:311:ILE:CG1	1:E:312:PRO:HD2	2.47	0.44
1:E:16:VAL:HB	1:E:20:VAL:O	2.18	0.44
1:F:311:ILE:O	1:F:312:PRO:C	2.55	0.44
1:E:280:ALA:HB2	1:E:290:ASN:OD1	2.17	0.44
1:A:318:MET:HB3	1:A:329:MET:SD	2.58	0.44
1:E:80:ASP:O	1:E:83:GLU:HG2	2.17	0.44
1:F:74:VAL:HA	1:F:79:VAL:O	2.17	0.44
1:B:210:ASP:HB2	3:B:3428:HOH:O	2.17	0.44
1:B:268:LYS:HE3	3:B:3252:HOH:O	2.17	0.44
1:F:36:LEU:HB2	3:F:3111:HOH:O	2.16	0.43
1:E:59:ALA:HB2	1:E:311:ILE:HB	2.00	0.43
1:F:80:ASP:O	1:F:83:GLU:HG2	2.18	0.43
1:E:75:GLN:NE2	1:E:266:ASP:N	2.62	0.43
1:D:48:MET:HE1	3:D:3329:HOH:O	2.19	0.43
1:D:201:ARG:O	1:D:333:ASN:HB2	2.18	0.43
1:D:74:VAL:HA	1:D:79:VAL:O	2.19	0.43
1:F:249:PRO:HB3	1:F:329:MET:O	2.18	0.43
1:C:269:ARG:N	1:C:269:ARG:HD2	2.34	0.42
1:C:126:THR:HG21	3:C:3314:HOH:O	2.19	0.42
1:F:75:GLN:CG	1:F:269:ARG:HD3	2.47	0.42
1:F:260:PHE:CG	1:F:320:ARG:HD2	2.55	0.42
1:C:344:LEU:HD12	1:C:344:LEU:HA	1.84	0.42
1:C:80:ASP:O	1:C:83:GLU:HG2	2.19	0.42
1:F:30:PRO:HG3	1:F:324:THR:O	2.19	0.42
1:F:260:PHE:CB	1:F:320:ARG:HD2	2.49	0.42
1:A:234:PHE:HA	1:A:235:PRO:HD2	1.75	0.42
1:C:75:GLN:CG	1:C:269:ARG:HD3	2.48	0.42
1:D:126:THR:HG23	3:D:3127:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:PHE:HB3	1:A:134:SER:OG	2.19	0.42
1:F:75:GLN:HE22	1:F:266:ASP:H	1.64	0.42
1:E:196:ILE:HG13	1:E:196:ILE:H	1.61	0.42
1:A:267:GLN:HE22	1:F:284:GLY:H	1.66	0.42
1:D:184:LYS:HE2	1:D:184:LYS:HB3	1.88	0.42
1:A:353:ARG:HG2	3:A:3370:HOH:O	2.19	0.42
1:A:136:ARG:NH2	3:A:3087:HOH:O	2.53	0.42
1:B:269:ARG:HD2	1:B:269:ARG:H	1.85	0.42
1:F:201:ARG:O	1:F:333:ASN:HB2	2.19	0.42
1:E:179:ALA:HB3	1:E:180:PRO:HD3	2.03	0.41
1:A:196:ILE:HD12	1:A:196:ILE:N	2.29	0.41
1:B:207:ALA:CB	1:B:210:ASP:HB3	2.49	0.41
1:F:25:LEU:HD13	1:F:330:LEU:HB2	2.01	0.41
1:A:162:ALA:HA	1:A:167:LYS:O	2.20	0.41
1:F:21:VAL:HG23	1:F:205:HIS:HE1	1.84	0.41
1:B:274:LYS:HB2	1:B:305:LYS:HD2	2.02	0.41
1:C:51:THR:H	1:C:54:HIS:CD2	2.19	0.41
1:F:204:MET:HA	1:F:205:HIS:CB	2.43	0.41
1:A:68:THR:HA	1:A:273:MET:HE1	2.03	0.41
1:D:283:PRO:HA	1:D:284:GLY:HA2	1.78	0.41
1:D:199:GLU:HG2	1:D:200:ALA:O	2.21	0.41
1:A:15:HIS:NE2	1:A:20:VAL:HG21	2.36	0.41
1:B:296:LEU:HD23	1:B:303:GLU:OE1	2.21	0.40
1:B:196:ILE:HG13	1:B:196:ILE:O	2.21	0.40
1:E:311:ILE:O	1:E:312:PRO:C	2.59	0.40
1:A:201:ARG:HD3	1:A:229:ASP:OD2	2.21	0.40
1:F:126:THR:HG21	3:F:3075:HOH:O	2.21	0.40
1:B:2:SER:HA	1:C:226:GLY:HA3	2.03	0.40
1:F:269:ARG:HD2	1:F:269:ARG:H	1.86	0.40
1:C:280:ALA:HB2	1:C:290:ASN:OD1	2.22	0.40

All (2) 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	Distance(Å)	Clash(Å)
3:B:3436:HOH:O	3:D:3163:HOH:O[1_655]	2.12	0.08
3:B:3448:HOH:O	3:C:3298:HOH:O[2_646]	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	360/363 (99%)	348 (97%)	11 (3%)	1 (0%)	50	49
1	B	362/363 (100%)	344 (95%)	14 (4%)	4 (1%)	21	13
1	C	354/363 (98%)	343 (97%)	10 (3%)	1 (0%)	50	49
1	D	346/363 (95%)	335 (97%)	10 (3%)	1 (0%)	50	49
1	E	339/363 (93%)	329 (97%)	7 (2%)	3 (1%)	25	17
1	F	321/363 (88%)	309 (96%)	10 (3%)	2 (1%)	33	28
All	All	2082/2178 (96%)	2008 (96%)	62 (3%)	12 (1%)	33	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	VAL
1	B	223	PRO
1	E	195	PRO
1	F	312	PRO
1	E	312	PRO
1	A	243	GLY
1	C	243	GLY
1	E	243	GLY
1	F	243	GLY
1	B	243	GLY
1	B	312	PRO
1	D	243	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	300/301 (100%)	291 (97%)	9 (3%)	53	55
1	B	302/301 (100%)	291 (96%)	11 (4%)	47	46
1	C	298/301 (99%)	288 (97%)	10 (3%)	49	49
1	D	290/301 (96%)	285 (98%)	5 (2%)	73	78
1	E	288/301 (96%)	281 (98%)	7 (2%)	61	65
1	F	272/301 (90%)	261 (96%)	11 (4%)	42	41
All	All	1750/1806 (97%)	1697 (97%)	53 (3%)	53	55

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	126	THR
1	A	196	ILE
1	A	265	LEU
1	A	307	HIS
1	A	320	ARG
1	A	329	MET
1	A	344	LEU
1	A	345	LYS
1	B	97	GLN
1	B	112	ASP
1	B	115	THR
1	B	116	SER
1	B	126	THR
1	B	216[A]	ASP
1	B	216[B]	ASP
1	B	224	VAL
1	B	269	ARG
1	B	307	HIS
1	B	329	MET
1	C	78	THR
1	C	86	THR
1	C	112	ASP
1	C	126	THR
1	C	227	VAL
1	C	236	LEU
1	C	269	ARG
1	C	307	HIS
1	C	329	MET
1	C	344	LEU

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Mol	Chain	Res	Type
1	D	119	MET
1	D	122	ASP
1	D	126	THR
1	D	184	LYS
1	D	329	MET
1	E	16	VAL
1	E	97	GLN
1	E	112	ASP
1	E	265	LEU
1	E	307	HIS
1	E	329	MET
1	E	353	ARG
1	F	23	VAL
1	F	117	MET
1	F	119	MET
1	F	124	SER
1	F	184	LYS
1	F	232	GLU
1	F	267	GLN
1	F	268	LYS
1	F	269	ARG
1	F	307	HIS
1	F	329	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	ASN
1	A	54	HIS
1	A	71	HIS
1	A	75	GLN
1	A	163	HIS
1	A	205	HIS
1	A	267	GLN
1	A	314	HIS
1	B	46	ASN
1	B	54	HIS
1	B	163	HIS
1	B	267	GLN
1	B	348	ASN
1	B	360	ASN

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Mol	Chain	Res	Type
1	C	54	HIS
1	C	75	GLN
1	C	267	GLN
1	C	348	ASN
1	C	360	ASN
1	D	6	ASN
1	D	54	HIS
1	D	163	HIS
1	D	360	ASN
1	E	54	HIS
1	E	75	GLN
1	E	97	GLN
1	E	205	HIS
1	E	360	ASN
1	F	54	HIS
1	F	75	GLN
1	F	205	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 23 ligands modelled in this entry, 23 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.

## 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 ⓘ

### 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	362/363 (99%)	-0.27	2 (0%) 86 90	11, 23, 36, 45	0
1	B	362/363 (99%)	-0.21	12 (3%) 44 49	10, 17, 46, 57	0
1	C	358/363 (98%)	-0.26	6 (1%) 67 71	10, 20, 40, 52	0
1	D	350/363 (96%)	-0.28	4 (1%) 77 81	9, 18, 36, 53	0
1	E	345/363 (95%)	0.16	17 (4%) 28 31	15, 31, 53, 64	0
1	F	327/363 (90%)	0.71	45 (13%) 4 4	15, 37, 56, 63	0
All	All	2104/2178 (96%)	-0.04	86 (4%) 35 40	9, 24, 50, 64	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	VAL	7.4
1	F	31	GLY	5.3
1	E	206	ALA	5.3
1	B	2	SER	5.3
1	F	41	TYR	5.2
1	B	363	SER	4.9
1	E	48	MET	4.9
1	F	40	GLY	4.8
1	C	363	SER	4.6
1	F	37	TYR	4.6
1	E	227	VAL	4.5
1	F	120	ILE	4.4
1	B	208	ALA	4.2
1	E	225	ASP	4.2
1	D	363	SER	4.2
1	B	212	ASN	4.1
1	F	344	LEU	4.1
1	F	11	ILE	4.1
1	E	41	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	196	ILE	3.7
1	F	115	THR	3.6
1	F	22	GLY	3.5
1	B	31	GLY	3.4
1	F	189	GLY	3.4
1	F	204	MET	3.4
1	F	228	TRP	3.2
1	B	3	ASP	3.1
1	F	20	VAL	3.0
1	F	48	MET	3.0
1	C	45	PHE	3.0
1	E	46	ASN	2.9
1	F	21	VAL	2.9
1	F	249	PRO	2.9
1	B	209	ASP	2.9
1	F	343	TYR	2.9
1	D	207	ALA	2.8
1	F	339	PHE	2.8
1	C	360	ASN	2.8
1	F	205	HIS	2.8
1	C	3	ASP	2.8
1	F	181	LEU	2.7
1	E	51	THR	2.7
1	B	207	ALA	2.7
1	F	35	SER	2.6
1	F	29	LEU	2.6
1	F	193	THR	2.6
1	B	362	ARG	2.6
1	F	233	TRP	2.5
1	B	216[A]	ASP	2.5
1	E	228	TRP	2.5
1	F	49	PRO	2.5
1	F	14	ASP	2.5
1	F	18	ARG	2.5
1	F	179	ALA	2.5
1	F	239	ALA	2.5
1	D	362	ARG	2.4
1	E	224	VAL	2.4
1	F	43	ASP	2.4
1	F	30	PRO	2.4
1	F	342	PHE	2.4
1	C	41	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	15	HIS	2.3
1	E	18	ARG	2.3
1	F	19	GLY	2.3
1	F	44	LYS	2.3
1	F	326	ALA	2.3
1	E	44	LYS	2.3
1	F	187	TRP	2.3
1	F	248	THR	2.3
1	E	198	ARG	2.2
1	F	312	PRO	2.2
1	E	49	PRO	2.2
1	F	337	GLY	2.2
1	E	47	LYS	2.1
1	F	346	GLY	2.1
1	F	353	ARG	2.1
1	E	226	GLY	2.1
1	C	5	ASN	2.1
1	F	232	GLU	2.1
1	B	45	PHE	2.1
1	F	55	LEU	2.1
1	D	115	THR	2.1
1	A	363	SER	2.1
1	A	224	VAL	2.0
1	E	203	TYR	2.0
1	E	343	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BA	F	3008	1/1	0.23	11.42	44,44,44,44	1
2	BA	A	3009	1/1	0.28	7.16	47,47,47,47	1
2	BA	B	3010	1/1	0.22	4.34	46,46,46,46	1
2	BA	D	3014	1/1	0.17	1.28	45,45,45,45	1
2	BA	B	3002	1/1	0.10	-0.15	43,43,43,43	1
2	BA	D	3013	1/1	0.12	-0.42	44,44,44,44	1
2	BA	D	3022	1/1	0.11	-0.92	55,55,55,55	1
2	BA	E	3012	1/1	0.09	-1.40	49,49,49,49	1
2	BA	F	3023	1/1	0.05	-1.92	70,70,70,70	1
2	BA	D	3017	1/1	0.07	-1.96	59,59,59,59	1
2	BA	A	3020	1/1	0.06	-2.18	52,52,52,52	1
2	BA	A	3004	1/1	0.07	-2.18	34,34,34,34	1
2	BA	F	3006	1/1	0.05	-2.28	43,43,43,43	1
2	BA	A	3003	1/1	0.04	-2.81	37,37,37,37	1
2	BA	E	3019	1/1	0.09	-3.06	56,56,56,56	1
2	BA	C	3011	1/1	0.04	-3.12	46,46,46,46	1
2	BA	C	3001	1/1	0.06	-3.12	34,34,34,34	1
2	BA	E	3018	1/1	0.06	-3.19	47,47,47,47	1
2	BA	F	3016	1/1	0.06	-3.38	72,72,72,72	1
2	BA	F	3007	1/1	0.11	-3.60	52,52,52,52	1
2	BA	C	3005	1/1	0.06	-5.93	20,20,20,20	1
2	BA	D	3015	1/1	0.05	-	45,45,45,45	1
2	BA	F	3021	1/1	0.10	-	76,76,76,76	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.