



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:49 PM GMT

PDB ID : 2DNS  
Title : The crystal structure of D-amino acid amidase from Ochrobactrum anthropi SV3 complexed with D-Phenylalanine  
Authors : Okazaki, S.; Suzuki, A.; Komeda, H.; Asano, Y.; Yamane, T.  
Deposited on : 2006-04-26  
Resolution : 2.40 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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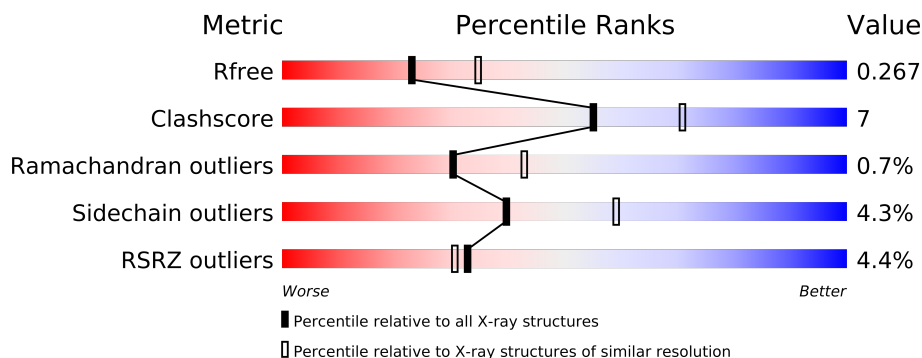
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17094 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.

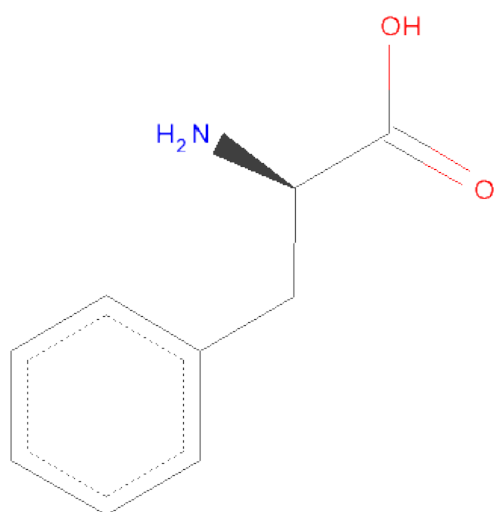
- Molecule 1 is a protein called D-amino acid amidase.

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	3	0
			2841	1791	496	538	16			
1	C	360	Total	C	N	O	S	0	0	0
			2799	1769	484	530	16			
1	D	355	Total	C	N	O	S	0	2	0
			2772	1756	479	519	18			
1	E	349	Total	C	N	O	S	0	0	0
			2709	1715	467	511	16			
1	F	300	Total	C	N	O	S	0	0	0
			2342	1483	405	439	15			

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

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

- Molecule 3 is D-PHENYLALANINE (three-letter code: DPN) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	9	1	1		
3	B	1	Total	C	N	O	0	0
			11	9	1	1		
3	C	1	Total	C	N	O	0	0
			11	9	1	1		
3	D	1	Total	C	N	O	0	0
			11	9	1	1		
3	E	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 4 is water.

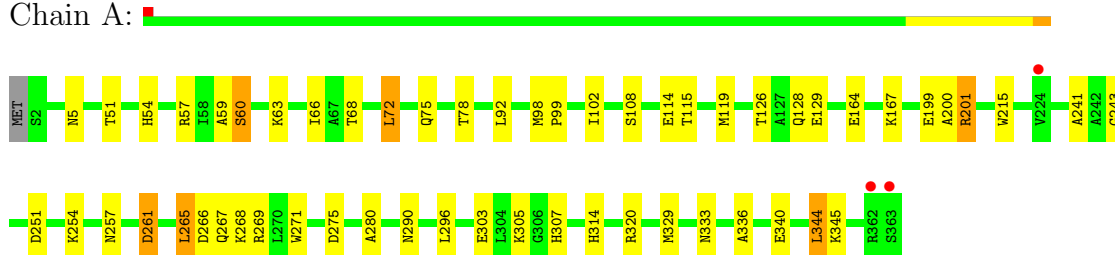
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	164	Total	O	0	0
			164	164		
4	C	158	Total	O	0	0
			158	158		
4	D	138	Total	O	0	0
			138	138		
4	E	70	Total	O	0	0
			70	70		
4	F	90	Total	O	0	0
			90	90		

### 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.

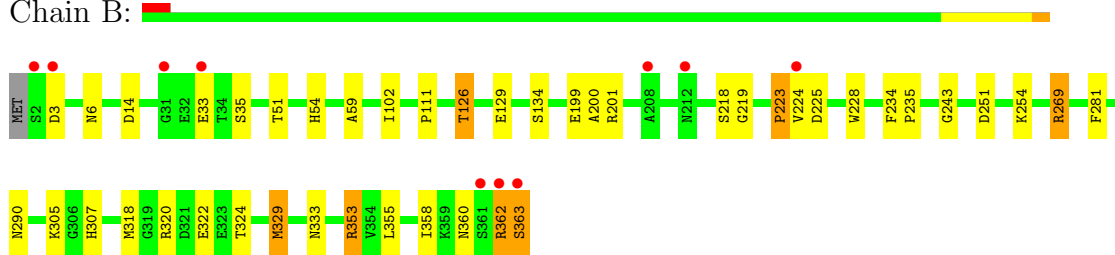
- Molecule 1: D-amino acid amidase

Chain A:



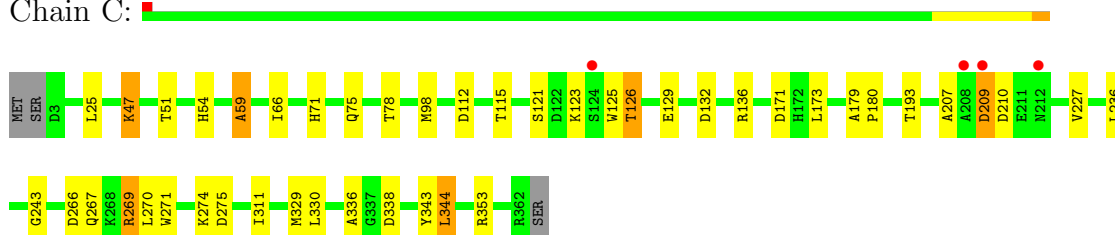
- Molecule 1: D-amino acid amidase

Chain B:



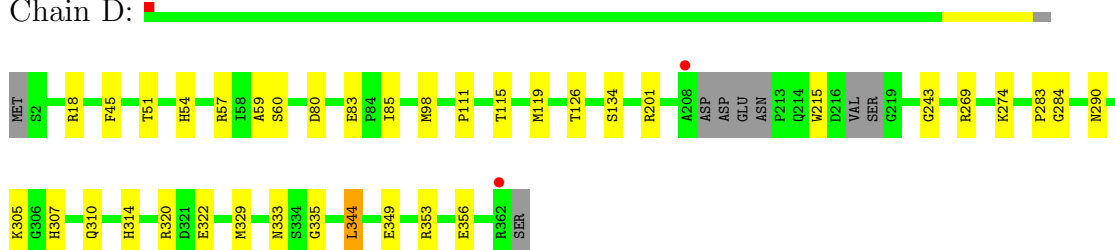
- Molecule 1: D-amino acid amidase

Chain C:



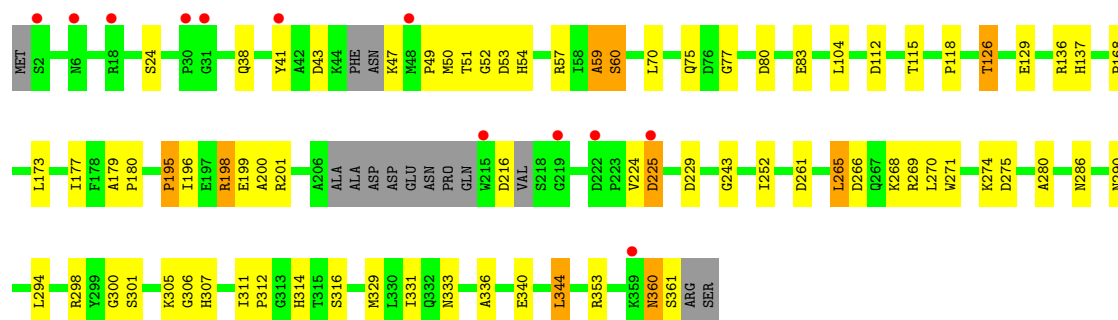
- Molecule 1: D-amino acid amidase

Chain D:



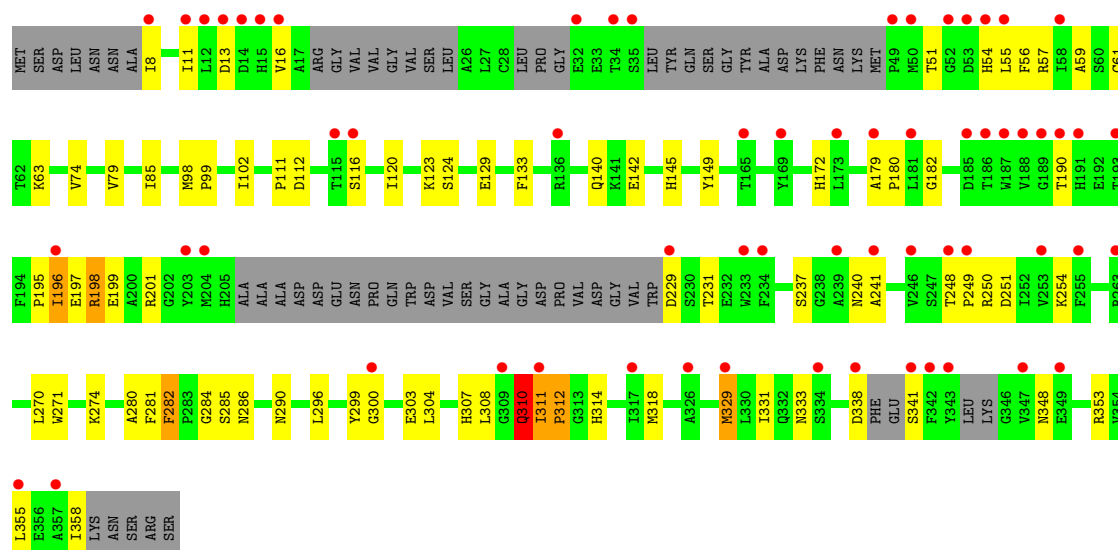
- Molecule 1: D-amino acid amidase

Chain E:



- Molecule 1: D-amino acid amidase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.07Å 123.70Å 116.05Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	19.87 – 2.40 19.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.87-2.40) 99.6 (19.87-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.195 , 0.269 0.195 , 0.267	Depositor DCC
$R_{free}$ test set	4106 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 17.9	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 81989 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: DPN, 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	0.47	0/2883	0.67	5/3910 (0.1%)
1	B	0.49	0/2913	0.68	3/3949 (0.1%)
1	C	0.48	0/2871	0.62	1/3894 (0.0%)
1	D	0.48	0/2845	0.67	5/3853 (0.1%)
1	E	0.44	0/2776	0.61	2/3759 (0.1%)
1	F	0.47	0/2397	0.59	0/3239
All	All	0.47	0/16685	0.64	16/22604 (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	B	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	ALA	C-N-CA	9.31	144.99	121.70
1	A	59	ALA	O-C-N	-9.24	107.92	122.70
1	D	59	ALA	O-C-N	-8.92	108.43	122.70
1	A	60	SER	O-C-N	-8.33	109.38	122.70
1	B	59	ALA	O-C-N	-8.28	109.45	122.70
1	B	59	ALA	C-N-CA	7.73	141.02	121.70
1	C	59	ALA	O-C-N	-7.10	111.35	122.70
1	A	59	ALA	CA-C-N	6.77	132.10	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	SER	CA-C-N	6.57	131.66	117.20
1	D	59	ALA	CA-C-N	6.49	131.47	117.20
1	E	60	SER	O-C-N	-6.27	112.67	122.70
1	A	59	ALA	C-N-CA	5.96	136.60	121.70
1	B	59	ALA	CA-C-N	5.95	130.30	117.20
1	E	59	ALA	O-C-N	-5.75	113.50	122.70
1	D	60	SER	O-C-N	-5.22	114.35	122.70
1	D	60	SER	CA-C-N	5.09	128.41	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	223	PRO	Peptide
1	E	60	SER	Mainchain

## 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	2709	38	0
1	B	2841	0	2739	26	0
1	C	2799	0	2700	32	0
1	D	2772	0	2687	20	0
1	E	2709	0	2620	40	0
1	F	2342	0	2266	58	0
2	A	5	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
3	A	11	0	10	1	0
3	B	11	0	10	0	0
3	C	11	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11	0	10	1	0
3	E	11	0	10	0	0
4	A	125	0	0	4	0
4	B	164	0	0	3	0
4	C	158	0	0	9	0
4	D	138	0	0	2	0
4	E	70	0	0	2	0
4	F	90	0	0	9	0
All	All	17094	0	15771	210	0

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 7.

All (210) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:102:ILE:HG21	4:A:3140:HOH:O	1.35	1.25
1:F:331:ILE:HG23	4:F:3090:HOH:O	1.52	1.06
1:A:267:GLN:NE2	1:F:284:GLY:H	1.60	0.98
1:A:51:THR:H	1:A:54:HIS:HD2	0.98	0.97
1:E:75:GLN:HE22	1:E:265:LEU:HA	1.32	0.91
1:A:267:GLN:HE22	1:F:284:GLY:H	0.94	0.91
1:A:51:THR:H	1:A:54:HIS:CD2	1.87	0.91
1:A:98:MET:HB3	1:A:102:ILE:HD11	1.52	0.91
1:C:75:GLN:HE22	1:C:266:ASP:H	1.19	0.89
1:C:126:THR:HG22	1:C:129:GLU:H	1.39	0.88
1:C:75:GLN:HG2	1:C:269:ARG:HD3	1.57	0.87
1:A:267:GLN:HE22	1:F:284:GLY:N	1.75	0.84
1:A:72:LEU:HD13	1:A:265:LEU:HD12	1.58	0.84
1:B:269:ARG:HD2	1:B:269:ARG:N	1.97	0.80
1:F:237:SER:HB3	4:F:3042:HOH:O	1.81	0.80
1:E:195:PRO:HB2	1:E:198:ARG:HG3	1.62	0.79
1:B:51:THR:H	1:B:54:HIS:HD2	1.28	0.79
1:C:126:THR:HG21	4:C:3091:HOH:O	1.82	0.78
1:E:51:THR:H	1:E:54:HIS:HD2	1.33	0.76
1:C:51:THR:H	1:C:54:HIS:HD2	1.30	0.75
1:D:57:ARG:H	1:D:314:HIS:HD2	1.32	0.75
1:D:51:THR:H	1:D:54:HIS:HD2	1.34	0.75
1:C:209:ASP:CB	4:C:3141:HOH:O	2.36	0.73
1:B:223:PRO:HD3	1:B:228:TRP:CZ2	2.24	0.72
1:C:75:GLN:HE22	1:C:266:ASP:N	1.88	0.71
1:B:51:THR:H	1:B:54:HIS:CD2	2.07	0.71
1:F:300:GLY:O	4:F:3089:HOH:O	2.08	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:240:ASN:CG	1:F:241:ALA:H	1.93	0.70
1:E:126:THR:HG22	1:E:129:GLU:H	1.56	0.70
1:C:75:GLN:NE2	1:C:266:ASP:H	1.89	0.70
1:A:257:ASN:O	1:A:261:ASP:HB2	1.90	0.70
1:F:57:ARG:H	1:F:314:HIS:HD2	1.40	0.69
1:F:59:ALA:HB2	1:F:311:ILE:HD13	1.74	0.69
1:C:336:ALA:H	1:C:344:LEU:HD13	1.56	0.69
1:E:80:ASP:O	1:E:83:GLU:HG2	1.92	0.68
1:C:209:ASP:HB3	4:C:3141:HOH:O	1.92	0.67
1:F:270:LEU:O	1:F:274:LYS:HG2	1.94	0.67
1:B:14:ASP:HB2	1:B:353[B]:ARG:HH22	1.59	0.66
1:A:75:GLN:NE2	1:A:266:ASP:H	1.93	0.66
1:E:75:GLN:NE2	1:E:266:ASP:H	1.94	0.64
1:A:126:THR:HB	1:A:129:GLU:HB2	1.79	0.64
1:D:119[A]:MET:CE	1:D:215:TRP:HB2	2.28	0.64
1:B:126:THR:HG22	1:B:129:GLU:H	1.62	0.64
1:E:118:PRO:HA	1:E:216:ASP:HB3	1.78	0.63
1:A:72:LEU:HD13	1:A:265:LEU:CD1	2.28	0.63
1:F:111:PRO:HG3	1:F:140:GLN:HB2	1.81	0.62
1:C:171:ASP:HB3	4:C:3160:HOH:O	1.99	0.62
1:F:195:PRO:HB2	1:F:198:ARG:HG3	1.82	0.62
1:F:190:THR:HB	4:F:3087:HOH:O	1.99	0.61
1:F:51:THR:H	1:F:54:HIS:CD2	2.18	0.61
1:E:24:SER:HB2	1:E:50:MET:HE2	1.82	0.61
1:C:209:ASP:HB2	4:C:3141:HOH:O	1.99	0.60
1:F:341:SER:N	4:F:3102:HOH:O	2.35	0.60
3:A:1060:DPN:C	4:A:3043:HOH:O	2.49	0.60
1:F:172:HIS:HA	4:F:3094:HOH:O	2.01	0.60
1:B:223:PRO:HB2	4:B:3121:HOH:O	2.02	0.60
1:F:51:THR:H	1:F:54:HIS:HD2	1.49	0.60
1:F:314:HIS:HB2	4:F:3073:HOH:O	2.03	0.59
1:F:280:ALA:HB2	1:F:290:ASN:OD1	2.03	0.59
1:E:201:ARG:O	1:E:333:ASN:HB2	2.03	0.59
1:B:224:VAL:HG23	1:B:225:ASP:HB3	1.84	0.59
1:F:355:LEU:O	1:F:358:ILE:HG22	2.04	0.58
1:A:99:PRO:O	1:A:102:ILE:HG13	2.04	0.58
1:F:61:CYS:HB3	1:F:318:MET:SD	2.43	0.58
1:B:269:ARG:HD2	1:B:269:ARG:H	1.70	0.56
1:B:126:THR:HG23	4:B:3058:HOH:O	2.04	0.56
1:F:286:ASN:ND2	1:F:299:TYR:CD1	2.74	0.56
1:A:126:THR:HG22	1:A:128:GLN:H	1.71	0.55
1:C:71:HIS:O	1:C:75:GLN:HG3	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:GLN:HE22	1:A:266:ASP:H	1.54	0.55
1:B:224:VAL:HG23	1:B:225:ASP:OD1	2.07	0.55
1:D:305:LYS:HE3	1:D:322:GLU:OE1	2.06	0.55
1:C:210:ASP:HA	1:C:338:ASP:HB2	1.89	0.55
1:D:119[A]:MET:HE2	1:D:215:TRP:HB2	1.89	0.54
1:D:45:PHE:HD1	4:D:3114:HOH:O	1.88	0.54
1:D:353:ARG:NH1	1:D:356:GLU:OE1	2.40	0.54
1:E:316:SER:HB3	1:E:331:ILE:HG23	1.89	0.54
1:E:38:GLN:NE2	1:E:52:GLY:HA2	2.22	0.54
1:A:75:GLN:HE22	1:A:265:LEU:HA	1.73	0.54
1:F:282:PHE:O	1:F:285:SER:OG	2.09	0.54
1:F:133:PHE:HD1	4:F:3037:HOH:O	1.91	0.53
1:D:201:ARG:O	1:D:333:ASN:HB2	2.08	0.53
1:C:179:ALA:HB3	1:C:180:PRO:HD3	1.89	0.53
1:B:111:PRO:O	1:B:134:SER:HB3	2.09	0.53
1:C:123:LYS:HD3	1:C:125:TRP:CE2	2.44	0.52
1:A:268:LYS:HD3	1:F:281:PHE:CD2	2.44	0.52
1:E:77:GLY:HA2	4:E:3040:HOH:O	2.09	0.52
1:E:75:GLN:NE2	1:E:265:LEU:HA	2.13	0.52
1:E:51:THR:H	1:E:54:HIS:CD2	2.21	0.52
1:B:320:ARG:HD3	4:B:3086:HOH:O	2.10	0.52
1:F:57:ARG:H	1:F:314:HIS:CD2	2.26	0.52
1:A:271:TRP:CD1	1:A:275:ASP:HB2	2.43	0.52
1:B:201:ARG:O	1:B:333:ASN:HB2	2.09	0.52
1:B:305:LYS:HE3	1:B:322:GLU:OE1	2.10	0.52
1:E:59:ALA:HB2	1:E:311:ILE:HB	1.90	0.52
1:F:59:ALA:CB	1:F:310:GLN:H	2.23	0.52
1:F:59:ALA:HB3	1:F:310:GLN:H	1.75	0.52
1:D:119[B]:MET:HE1	3:D:1060:DPN:HE2	1.92	0.51
1:F:201:ARG:HB3	1:F:229:ASP:OD2	2.11	0.51
1:C:132:ASP:O	1:C:136:ARG:HG3	2.09	0.51
1:A:126:THR:HG22	1:A:128:GLN:N	2.26	0.51
1:E:224:VAL:O	1:E:225:ASP:HB2	2.11	0.51
1:B:33:GLU:HB2	1:C:209:ASP:OD1	2.10	0.51
1:F:54:HIS:O	1:F:248:THR:HG22	2.11	0.51
1:D:119[A]:MET:HG3	1:D:215:TRP:HB3	1.94	0.51
1:F:355:LEU:HG	4:F:3026:HOH:O	2.10	0.50
1:A:340:GLU:OE2	4:A:3142:HOH:O	2.19	0.50
1:F:285:SER:HA	1:F:348:ASN:HD21	1.76	0.50
1:F:13:ASP:HA	1:F:16:VAL:HG22	1.93	0.50
1:F:251:ASP:HA	1:F:254:LYS:HD2	1.93	0.50
1:E:271:TRP:CD1	1:E:275:ASP:HB2	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:240:ASN:CG	1:F:241:ALA:N	2.64	0.50
3:C:1060:DPN:C	4:C:3074:HOH:O	2.59	0.50
1:E:201:ARG:HD3	1:E:229:ASP:OD2	2.12	0.50
1:C:266:ASP:OD1	1:C:269:ARG:HD2	2.12	0.49
1:D:310:GLN:NE2	1:D:344:LEU:HG	2.27	0.49
1:F:63:LYS:HD2	1:F:149:TYR:OH	2.12	0.49
1:E:75:GLN:HE22	1:E:265:LEU:CA	2.15	0.49
1:C:59:ALA:HB2	1:C:311:ILE:HB	1.94	0.49
1:B:324:THR:HG22	1:B:362:ARG:HH12	1.78	0.49
1:B:225:ASP:OD2	1:B:225:ASP:O	2.31	0.48
1:E:280:ALA:HB2	1:E:290:ASN:OD1	2.13	0.48
1:A:57:ARG:H	1:A:314:HIS:HD2	1.60	0.48
1:F:142:GLU:O	1:F:145:HIS:HB3	2.14	0.48
1:A:68:THR:HG23	1:A:265:LEU:HD13	1.96	0.48
1:D:111:PRO:O	1:D:134:SER:HB3	2.13	0.48
1:D:274:LYS:HD2	1:D:322:GLU:OE2	2.14	0.48
1:B:360:ASN:HA	1:B:363:SER:HB2	1.96	0.48
1:F:85:ILE:HG12	1:F:98:MET:HB2	1.95	0.48
1:A:78:THR:OG1	1:A:164:GLU:OE1	2.32	0.47
1:C:98:MET:HE2	4:C:3012:HOH:O	2.14	0.47
1:A:280:ALA:HB2	1:A:290:ASN:OD1	2.15	0.47
1:E:270:LEU:O	1:E:274:LYS:HG2	2.13	0.47
1:A:257:ASN:HA	1:A:320:ARG:HH21	1.79	0.47
1:A:201:ARG:O	1:A:333:ASN:HB2	2.14	0.47
1:F:299:TYR:HE2	1:F:304:LEU:HD12	1.81	0.46
1:C:66:ILE:HD13	1:C:173:LEU:HD11	1.97	0.46
1:D:80:ASP:O	1:D:83:GLU:HG2	2.14	0.46
1:F:56:PHE:HE1	1:F:333:ASN:OD1	1.99	0.46
1:E:173:LEU:O	1:E:177:ILE:HB	2.16	0.46
4:C:3144:HOH:O	1:E:300:GLY:HA2	2.16	0.46
1:E:126:THR:HG21	4:E:3074:HOH:O	2.15	0.46
1:B:199:GLU:HG2	1:B:200:ALA:O	2.16	0.46
1:F:249:PRO:HB3	1:F:329:MET:O	2.15	0.45
1:A:251:ASP:O	1:A:254:LYS:HB2	2.15	0.45
1:E:252:ILE:HG21	1:E:329:MET:HE2	1.99	0.45
1:F:311:ILE:HB	1:F:312:PRO:HD2	1.98	0.45
1:F:123:LYS:HZ1	1:F:129:GLU:CD	2.20	0.45
1:E:360:ASN:O	1:E:361:SER:HB2	2.17	0.45
1:F:251:ASP:O	1:F:254:LYS:HB2	2.17	0.45
1:F:98:MET:HB3	1:F:102:ILE:HG21	1.98	0.44
1:C:98:MET:CE	4:C:3012:HOH:O	2.65	0.44
1:A:66:ILE:HG13	1:A:241:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:179:ALA:N	1:F:180:PRO:HD2	2.32	0.44
1:E:199:GLU:HG2	1:E:200:ALA:O	2.17	0.44
1:E:57:ARG:H	1:E:314:HIS:HD2	1.66	0.44
1:A:336:ALA:H	1:A:344:LEU:HD13	1.82	0.44
1:F:8:ILE:HA	1:F:11:ILE:HD12	2.00	0.43
1:E:43:ASP:O	1:E:47:LYS:HA	2.17	0.43
1:F:55:LEU:H	1:F:199:GLU:HA	1.82	0.43
1:B:355:LEU:HA	1:B:358:ILE:HD12	1.99	0.43
1:A:102:ILE:O	1:A:108:SER:HB3	2.18	0.43
1:E:57:ARG:H	1:E:314:HIS:CD2	2.36	0.43
1:E:41:TYR:HA	1:E:49:PRO:HA	2.00	0.43
1:E:179:ALA:HB3	1:E:180:PRO:HD3	2.00	0.43
1:F:296:LEU:HD11	1:F:303:GLU:HB2	2.01	0.43
1:D:283:PRO:HA	1:D:284:GLY:HA2	1.84	0.43
1:F:57:ARG:N	1:F:314:HIS:HD2	2.10	0.43
1:F:286:ASN:ND2	1:F:299:TYR:CE1	2.86	0.43
1:F:250:ARG:HG2	1:F:254:LYS:HE3	2.00	0.43
1:D:274:LYS:O	1:D:305:LYS:NZ	2.52	0.42
1:C:123:LYS:HD3	1:C:125:TRP:CZ2	2.54	0.42
1:D:85:ILE:HD11	1:D:98:MET:HE2	2.01	0.42
1:D:57:ARG:N	1:D:314:HIS:HD2	2.09	0.42
1:C:207:ALA:O	1:C:343:TYR:CE2	2.72	0.42
1:A:119:MET:HG3	1:A:215:TRP:HB3	2.02	0.42
1:E:286:ASN:HB3	1:E:298:ARG:O	2.19	0.42
1:F:338:ASP:O	1:F:341:SER:HB3	2.19	0.42
1:F:56:PHE:CE1	1:F:333:ASN:OD1	2.73	0.42
1:F:56:PHE:CG	1:F:331:ILE:HG21	2.54	0.42
1:A:296:LEU:HD13	1:A:305:LYS:HG2	2.01	0.42
1:B:234:PHE:HA	1:B:235:PRO:HD3	1.93	0.41
1:B:251:ASP:O	1:B:254:LYS:HB3	2.20	0.41
1:A:75:GLN:HE21	1:A:269:ARG:HB2	1.84	0.41
1:A:199:GLU:HG2	1:A:200:ALA:O	2.19	0.41
1:E:136:ARG:HG2	1:E:137:HIS:CE1	2.55	0.41
1:E:118:PRO:HA	1:E:216:ASP:CB	2.46	0.41
1:C:271:TRP:CD1	1:C:275:ASP:HB2	2.55	0.41
1:C:25:LEU:HD13	1:C:330:LEU:HD12	2.02	0.41
1:A:60:SER:O	1:A:63:LYS:HB2	2.20	0.41
1:E:265:LEU:HG	1:E:269:ARG:HB3	2.02	0.41
1:E:70:LEU:HD23	1:E:104:LEU:HD11	2.03	0.41
1:E:38:GLN:HE21	1:E:52:GLY:HA2	1.84	0.41
1:A:296:LEU:HD11	1:A:303:GLU:OE2	2.21	0.41
1:A:114:GLU:HG2	4:A:3051:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:335:GLY:HA3	4:D:3081:HOH:O	2.20	0.41
1:E:336:ALA:H	1:E:344:LEU:HD13	1.86	0.41
1:F:74:VAL:HA	1:F:79:VAL:O	2.21	0.41
1:C:47:LYS:HD3	1:C:47:LYS:HA	1.91	0.41
1:B:318:MET:HB3	1:B:329:MET:SD	2.61	0.41
1:C:75:GLN:HE21	1:C:269:ARG:HB2	1.86	0.40
1:C:51:THR:H	1:C:54:HIS:CD2	2.22	0.40
1:F:99:PRO:O	1:F:102:ILE:HG22	2.21	0.40
1:E:294:LEU:HD22	1:E:306:GLY:HA2	2.02	0.40
1:A:265:LEU:HG	1:A:269:ARG:HB3	2.02	0.40
1:B:218:SER:HA	1:B:219:GLY:HA2	1.89	0.40
1:D:18:ARG:NH1	1:D:349:GLU:OE1	2.55	0.40
1:C:353:ARG:HD3	1:C:353:ARG:HA	1.97	0.40
1:B:281:PHE:HB2	1:F:271:TRP:CE2	2.56	0.40
1:C:270:LEU:HG	1:C:274:LYS:HE3	2.04	0.40

There are no symmetry-related clashes.

## 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%)	349 (97%)	10 (3%)	1 (0%)	50	68
1	B	363/363 (100%)	346 (95%)	16 (4%)	1 (0%)	50	68
1	C	358/363 (99%)	341 (95%)	15 (4%)	2 (1%)	33	47
1	D	351/363 (97%)	338 (96%)	12 (3%)	1 (0%)	50	68
1	E	341/363 (94%)	322 (94%)	14 (4%)	5 (2%)	15	20
1	F	286/363 (79%)	264 (92%)	17 (6%)	5 (2%)	14	17
All	All	2059/2178 (94%)	1960 (95%)	84 (4%)	15 (1%)	30	43

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	310	GLN
1	E	360	ASN
1	F	182	GLY
1	A	243	GLY
1	E	243	GLY
1	F	312	PRO
1	B	243	GLY
1	C	47	LYS
1	C	243	GLY
1	F	197	GLU
1	F	196	ILE
1	D	243	GLY
1	E	168	PRO
1	E	195	PRO
1	E	312	PRO

### 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%)	288 (96%)	12 (4%)	42	63
1	B	303/301 (101%)	290 (96%)	13 (4%)	40	59
1	C	298/301 (99%)	285 (96%)	13 (4%)	39	58
1	D	295/301 (98%)	287 (97%)	8 (3%)	57	78
1	E	289/301 (96%)	273 (94%)	16 (6%)	30	46
1	F	251/301 (83%)	237 (94%)	14 (6%)	30	45
All	All	1736/1806 (96%)	1660 (96%)	76 (4%)	40	58

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	72	LEU
1	A	92	LEU
1	A	115	THR
1	A	167	LYS

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Mol	Chain	Res	Type
1	A	201	ARG
1	A	261	ASP
1	A	265	LEU
1	A	307	HIS
1	A	329	MET
1	A	344	LEU
1	A	345	LYS
1	B	3	ASP
1	B	6	ASN
1	B	35	SER
1	B	102	ILE
1	B	126	THR
1	B	269	ARG
1	B	290	ASN
1	B	307	HIS
1	B	329	MET
1	B	353[A]	ARG
1	B	353[B]	ARG
1	B	362	ARG
1	B	363	SER
1	C	78	THR
1	C	112	ASP
1	C	115	THR
1	C	121	SER
1	C	126	THR
1	C	193	THR
1	C	209	ASP
1	C	227	VAL
1	C	236	LEU
1	C	267	GLN
1	C	269	ARG
1	C	329	MET
1	C	344	LEU
1	D	115	THR
1	D	126	THR
1	D	269	ARG
1	D	290	ASN
1	D	307	HIS
1	D	320	ARG
1	D	329	MET
1	D	344	LEU
1	E	53	ASP

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Mol	Chain	Res	Type
1	E	112	ASP
1	E	115	THR
1	E	126	THR
1	E	196	ILE
1	E	198	ARG
1	E	225	ASP
1	E	261	ASP
1	E	265	LEU
1	E	268	LYS
1	E	301	SER
1	E	305	LYS
1	E	307	HIS
1	E	340	GLU
1	E	344	LEU
1	E	353	ARG
1	F	112	ASP
1	F	116	SER
1	F	120	ILE
1	F	124	SER
1	F	196	ILE
1	F	198	ARG
1	F	231	THR
1	F	282	PHE
1	F	307	HIS
1	F	308	LEU
1	F	310	GLN
1	F	311	ILE
1	F	329	MET
1	F	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	54	HIS
1	A	75	GLN
1	A	163	HIS
1	A	205	HIS
1	A	212	ASN
1	A	267	GLN
1	A	360	ASN
1	B	46	ASN

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Mol	Chain	Res	Type
1	B	54	HIS
1	B	267	GLN
1	B	348	ASN
1	B	360	ASN
1	C	5	ASN
1	C	54	HIS
1	C	75	GLN
1	C	163	HIS
1	C	267	GLN
1	D	6	ASN
1	D	54	HIS
1	D	314	HIS
1	D	360	ASN
1	E	5	ASN
1	E	54	HIS
1	E	75	GLN
1	E	205	HIS
1	E	314	HIS
1	F	9	GLN
1	F	54	HIS
1	F	75	GLN
1	F	163	HIS
1	F	191	HIS
1	F	205	HIS
1	F	314	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 25 ligands modelled in this entry, 20 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DPN	A	1060	1	11,11,12	4.96	1 (9%)	11,13,15	1.70	1 (9%)
3	DPN	B	1060	1	11,11,12	4.93	1 (9%)	11,13,15	1.72	1 (9%)
3	DPN	C	1060	1	11,11,12	4.75	1 (9%)	11,13,15	1.04	1 (9%)
3	DPN	D	1060	1	11,11,12	5.29	1 (9%)	11,13,15	0.89	1 (9%)
3	DPN	E	1060	1	11,11,12	4.99	1 (9%)	11,13,15	1.06	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DPN	A	1060	1	-	0/4/6/8	0/1/1/1
3	DPN	B	1060	1	-	0/4/6/8	0/1/1/1
3	DPN	C	1060	1	-	0/4/6/8	0/1/1/1
3	DPN	D	1060	1	-	0/4/6/8	0/1/1/1
3	DPN	E	1060	1	-	0/4/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1060	DPN	O-C	17.40	1.23	1.11
3	E	1060	DPN	O-C	16.45	1.22	1.11
3	A	1060	DPN	O-C	16.31	1.22	1.11
3	B	1060	DPN	O-C	16.27	1.22	1.11
3	C	1060	DPN	O-C	15.61	1.22	1.11

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1060	DPN	C-CA-N	-5.33	108.51	113.83
3	B	1060	DPN	C-CA-N	-5.30	108.53	113.83
3	D	1060	DPN	C-CA-N	-2.45	111.38	113.83
3	E	1060	DPN	C-CA-N	-2.20	111.63	113.83
3	C	1060	DPN	C-CA-N	-2.09	111.74	113.83

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%)	-0.22	3 (0%) 83 82	14, 29, 40, 55	0
1	B	362/363 (99%)	-0.24	10 (2%) 50 48	14, 23, 41, 56	0
1	C	360/363 (99%)	-0.33	4 (1%) 77 77	13, 24, 42, 49	0
1	D	355/363 (97%)	-0.30	2 (0%) 86 86	12, 23, 40, 61	0
1	E	349/363 (96%)	0.16	12 (3%) 43 41	18, 37, 58, 74	0
1	F	300/363 (82%)	1.04	62 (20%) 1 1	22, 53, 70, 72	0
All	All	2088/2178 (95%)	-0.01	93 (4%) 33 30	12, 28, 59, 74	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	SER	6.4
1	E	31	GLY	5.7
1	D	208	ALA	5.6
1	F	239	ALA	4.5
1	F	193	THR	4.4
1	F	233	TRP	4.3
1	F	189	GLY	4.2
1	F	248	THR	4.2
1	C	208	ALA	4.0
1	F	204	MET	4.0
1	A	363	SER	3.9
1	F	115	THR	3.9
1	F	12	LEU	3.7
1	F	342	PHE	3.6
1	B	2	SER	3.6
1	F	50	MET	3.5
1	F	196	ILE	3.5
1	F	334	SER	3.4
1	F	11	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	224	VAL	3.3
1	B	362	ARG	3.3
1	F	55	LEU	3.2
1	F	34	THR	3.2
1	F	187	TRP	3.2
1	F	15	HIS	3.2
1	F	203	TYR	3.2
1	F	253	VAL	3.2
1	E	48	MET	3.0
1	F	246	VAL	3.0
1	F	326	ALA	3.0
1	B	31	GLY	3.0
1	F	186	THR	3.0
1	F	35	SER	3.0
1	F	343	TYR	2.9
1	F	190	THR	2.9
1	F	188	VAL	2.9
1	F	54	HIS	2.8
1	F	58	ILE	2.7
1	F	49	PRO	2.7
1	E	219	GLY	2.7
1	B	361	SER	2.7
1	F	249	PRO	2.7
1	F	300	GLY	2.7
1	F	357	ALA	2.7
1	F	181	LEU	2.6
1	F	8	ILE	2.6
1	F	136	ARG	2.6
1	E	6	ASN	2.5
1	E	2	SER	2.5
1	F	16	VAL	2.5
1	F	32	GLU	2.5
1	F	14	ASP	2.5
1	C	124	SER	2.5
1	C	209	ASP	2.5
1	E	215	TRP	2.5
1	F	347	VAL	2.4
1	E	222	ASP	2.4
1	F	116	SER	2.4
1	B	208	ALA	2.4
1	F	341	SER	2.4
1	E	225	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	338	ASP	2.3
1	B	212	ASN	2.3
1	F	165	THR	2.3
1	B	33	GLU	2.3
1	E	359	LYS	2.3
1	F	355	LEU	2.3
1	F	13	ASP	2.3
1	F	185	ASP	2.3
1	F	317	ILE	2.3
1	F	173	LEU	2.2
1	E	30	PRO	2.2
1	F	229	ASP	2.2
1	F	241	ALA	2.2
1	F	53	ASP	2.2
1	A	362	ARG	2.2
1	F	169	TYR	2.2
1	F	329	MET	2.2
1	C	212	ASN	2.2
1	F	179	ALA	2.1
1	E	41	TYR	2.1
1	F	52	GLY	2.1
1	F	255	PHE	2.1
1	F	311	ILE	2.1
1	B	3	ASP	2.1
1	F	191	HIS	2.1
1	D	362	ARG	2.1
1	A	224	VAL	2.0
1	F	349	GLU	2.0
1	F	234	PHE	2.0
1	E	18	ARG	2.0
1	F	263	ARG	2.0
1	F	309	GLY	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(Å <sup>2</sup> )	Q<0.9
3	DPN	A	1060	11/12	0.15	1.47	22,23,24,26	0
3	DPN	D	1060	11/12	0.16	0.54	29,31,33,34	0
3	DPN	C	1060	11/12	0.11	0.16	13,16,19,19	0
3	DPN	E	1060	11/12	0.14	0.12	28,31,32,32	0
3	DPN	B	1060	11/12	0.11	0.10	23,26,27,27	0
2	BA	E	3016	1/1	0.10	-1.45	36,36,36,36	1
2	BA	A	3003	1/1	0.05	-1.54	28,28,28,28	1
2	BA	A	3018	1/1	0.07	-1.60	57,57,57,57	1
2	BA	A	3020	1/1	0.10	-2.25	66,66,66,66	1
2	BA	D	3012	1/1	0.18	-2.29	61,61,61,61	1
2	BA	A	3007	1/1	0.12	-2.61	59,59,59,59	1
2	BA	C	3005	1/1	0.01	-2.62	37,37,37,37	1
2	BA	F	3008	1/1	0.13	-2.81	49,49,49,49	1
2	BA	B	3019	1/1	0.11	-2.92	59,59,59,59	1
2	BA	F	3014	1/1	0.08	-2.99	44,44,44,44	1
2	BA	D	3017	1/1	0.06	-3.01	58,58,58,58	1
2	BA	A	3004	1/1	0.04	-3.53	41,41,41,41	1
2	BA	D	3015	1/1	0.07	-3.86	29,29,29,29	1
2	BA	C	3011	1/1	0.06	-4.47	53,53,53,53	1
2	BA	C	3009	1/1	0.15	-4.58	71,71,71,71	1
2	BA	C	3001	1/1	0.04	-4.66	29,29,29,29	0
2	BA	F	3006	1/1	0.06	-5.22	51,51,51,51	1
2	BA	B	3002	1/1	0.04	-5.49	28,28,28,28	1
2	BA	D	3013	1/1	0.06	-8.33	59,59,59,59	1
2	BA	E	3010	1/1	0.06	-12.62	73,73,73,73	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.