



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:49 AM GMT

PDB ID : 2EFU  
Title : The crystal structure of D-amino acid amidase from Ochrobactrum anthropi SV3 complexed with L-phenylalanine  
Authors : Okazaki, S.; Suzuki, A.; Mizushima, T.; Komeda, H.; Asano, Y.; Yamane, T.  
Deposited on : 2007-02-26  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

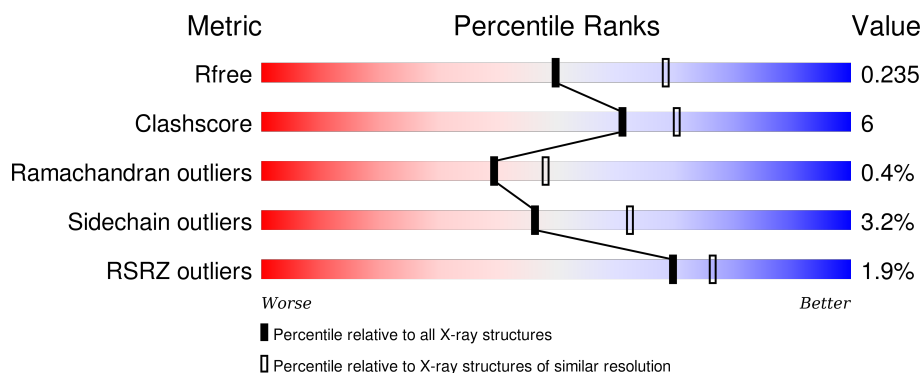
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	363	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	363	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	363	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
1	D	363	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	E	363	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>.</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	363	 2% 78% 12% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PHE	C	2003	-	-	-	X
3	PHE	E	2005	-	-	-	X
3	PHE	F	2006	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17915 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.

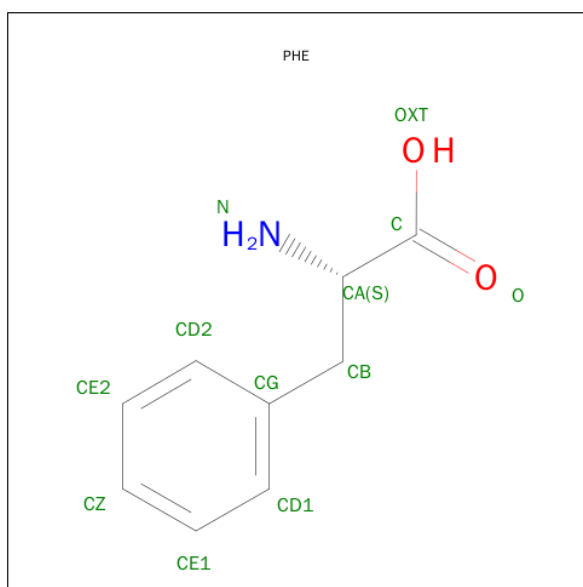
- Molecule 1 is a protein called D-Amino acid amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	1	0
			2819	1780	487	535	17			
1	B	359	Total	C	N	O	S	0	2	0
			2806	1774	484	531	17			
1	C	361	Total	C	N	O	S	0	0	0
			2805	1772	485	532	16			
1	D	350	Total	C	N	O	S	0	1	0
			2726	1725	474	511	16			
1	E	342	Total	C	N	O	S	0	0	0
			2665	1688	462	499	16			
1	F	330	Total	C	N	O	S	0	2	0
			2589	1644	447	482	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	5	Total	Ba	0	1
			6	6		
2	E	4	Total	Ba	0	0
			4	4		
2	B	2	Total	Ba	0	0
			2	2		
2	C	4	Total	Ba	0	0
			4	4		
2	A	4	Total	Ba	0	0
			4	4		
2	F	6	Total	Ba	0	0
			6	6		

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

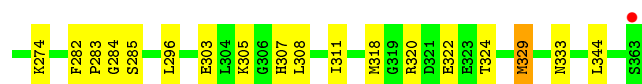


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	B	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		
3	D	1	Total	C	N	O	0	0
			12	9	1	2		
3	E	1	Total	C	N	O	0	0
			12	9	1	2		
3	F	1	Total	C	N	O	0	0
			12	9	1	2		

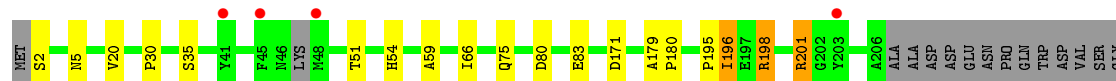
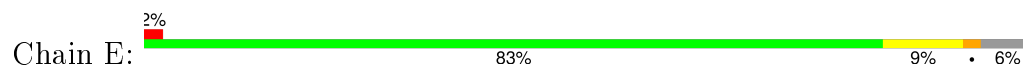
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	B	304	Total	O	0	0
			304	304		
4	C	248	Total	O	0	0
			248	248		
4	D	255	Total	O	0	0
			255	255		
4	E	198	Total	O	0	0
			198	198		
4	F	179	Total	O	0	0
			179	179		

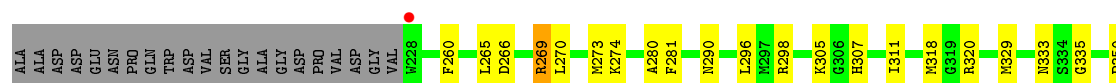
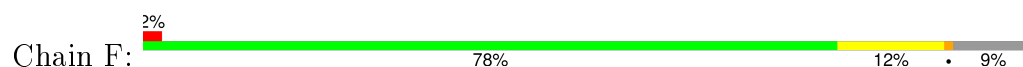




- Molecule 1: D-Amino acid amidase



- Molecule 1: D-Amino acid amidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.47Å 123.27Å 116.16Å 90.00° 104.05° 90.00°	Depositor
Resolution (Å)	47.67 – 2.30 47.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-2.30) 100.0 (47.66-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.170 , 0.235 0.170 , 0.235	Depositor DCC
$R_{free}$ test set	4735 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 93906 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.46	0/2891	0.59	0/3921
1	B	0.53	0/2880	0.65	1/3904 (0.0%)
1	C	0.49	0/2877	0.61	0/3902
1	D	0.50	0/2797	0.60	0/3788
1	E	0.46	0/2731	0.56	0/3697
1	F	0.49	0/2660	0.61	1/3602 (0.0%)
All	All	0.49	0/16836	0.61	2/22814 (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	2
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	114	GLU	N-CA-C	-7.49	90.78	111.00
1	B	226	GLY	N-CA-C	-5.01	100.56	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	224	VAL	Peptide
1	B	225	ASP	Peptide
1	F	113	PHE	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	2819	0	2719	32	0
1	B	2806	0	2711	26	0
1	C	2805	0	2706	26	0
1	D	2726	0	2651	31	0
1	E	2665	0	2587	31	0
1	F	2589	0	2522	39	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	1	0
2	D	6	0	0	0	0
2	E	4	0	0	0	0
2	F	6	0	0	0	0
3	A	12	0	8	0	0
3	B	12	0	8	0	0
3	C	12	0	8	0	0
3	D	12	0	8	0	0
3	E	12	0	8	0	0
3	F	12	0	8	0	0
4	A	223	0	0	4	0
4	B	304	0	0	7	0
4	C	248	0	0	4	0
4	D	255	0	0	2	0
4	E	198	0	0	1	0
4	F	179	0	0	4	0
All	All	17915	0	15944	177	0

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 6.

All (177) 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)
2:C:3001:BA:BA	4:C:3068:HOH:O	1.25	1.27
1:F:265:LEU:CD1	1:F:273:MET:CE	2.38	1.02
1:A:353:ARG:NH1	4:A:3239:HOH:O	1.92	1.02
1:F:265:LEU:HD12	1:F:273:MET:CE	1.92	0.99
1:A:51:THR:H	1:A:54:HIS:HD2	1.05	0.97
1:F:204:MET:HA	1:F:205:HIS:HB2	1.52	0.92
1:A:353:ARG:HG2	4:A:3240:HOH:O	1.72	0.89
1:A:51:THR:H	1:A:54:HIS:CD2	1.92	0.86
1:E:51:THR:H	1:E:54:HIS:HD2	1.21	0.86
1:C:51:THR:H	1:C:54:HIS:HD2	1.23	0.84
1:D:284:GLY:HA2	1:E:267:GLN:OE1	1.78	0.83
1:B:51:THR:H	1:B:54:HIS:HD2	1.25	0.83
1:F:51:THR:H	1:F:54:HIS:HD2	1.25	0.81
1:F:265:LEU:CD1	1:F:273:MET:HE2	2.09	0.81
1:F:265:LEU:HD11	1:F:273:MET:CE	2.09	0.81
1:D:51:THR:H	1:D:54:HIS:HD2	1.28	0.80
1:C:126:THR:HG22	1:C:129:GLU:H	1.46	0.80
1:A:141:LYS:HE2	4:A:3105:HOH:O	1.84	0.77
1:E:75:GLN:NE2	1:E:266:ASP:H	1.83	0.76
1:F:265:LEU:CD1	1:F:273:MET:HE1	2.16	0.75
1:C:210:ASP:HA	1:C:338:ASP:HB2	1.70	0.73
1:A:72:LEU:HD13	1:A:265:LEU:HD12	1.71	0.72
1:E:171:ASP:HB3	4:E:3125:HOH:O	1.88	0.71
1:E:75:GLN:HE22	1:E:265:LEU:HA	1.55	0.70
1:D:284:GLY:CA	1:E:267:GLN:OE1	2.39	0.70
1:C:267:GLN:HE22	1:E:284:GLY:H	1.37	0.70
1:F:265:LEU:HD12	1:F:273:MET:HE3	1.73	0.69
1:C:75:GLN:HE22	1:C:265:LEU:HA	1.58	0.69
1:F:265:LEU:HD11	1:F:273:MET:HE2	1.74	0.68
1:A:225:ASP:OD1	1:D:2:SER:N	2.27	0.68
1:B:51:THR:H	1:B:54:HIS:CD2	2.10	0.68
1:F:265:LEU:HD11	1:F:273:MET:HE1	1.75	0.68
1:D:296:LEU:CD2	1:D:305:LYS:HD3	2.24	0.68
1:A:71:HIS:HD2	1:A:273:MET:CE	2.08	0.67
1:E:195:PRO:HB2	1:E:198:ARG:HG3	1.77	0.66
1:F:75:GLN:HE22	1:F:265:LEU:HA	1.61	0.65
1:E:75:GLN:HE22	1:E:266:ASP:H	1.44	0.65
1:B:269:ARG:HD2	1:B:269:ARG:N	2.12	0.64
1:B:167:LYS:HE3	4:B:3196:HOH:O	1.95	0.64
1:C:196:ILE:HG22	4:C:3114:HOH:O	1.98	0.63
1:D:296:LEU:HD22	1:D:305:LYS:HD3	1.80	0.63
1:A:57:ARG:H	1:A:314:HIS:HD2	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:THR:H	1:F:54:HIS:CD2	2.12	0.62
1:D:51:THR:H	1:D:54:HIS:CD2	2.16	0.62
1:B:214:GLN:HG2	1:B:337:GLY:O	2.00	0.62
1:F:270:LEU:O	1:F:274:LYS:HG2	2.00	0.61
1:E:51:THR:H	1:E:54:HIS:CD2	2.12	0.60
1:C:336:ALA:H	1:C:344:LEU:HD13	1.67	0.60
1:F:80:ASP:O	1:F:83:GLU:HG2	2.02	0.60
1:F:75:GLN:HG3	1:F:269:ARG:HD3	1.84	0.59
1:C:267:GLN:NE2	1:E:284:GLY:H	1.99	0.59
1:F:126:THR:HG21	4:F:3083:HOH:O	2.02	0.59
1:F:126:THR:HG22	1:F:129:GLU:H	1.68	0.59
1:C:75:GLN:NE2	1:C:266:ASP:H	2.02	0.58
1:A:75:GLN:NE2	1:A:266:ASP:H	2.01	0.58
1:C:51:THR:H	1:C:54:HIS:CD2	2.14	0.58
1:D:48:MET:HG3	4:D:3221:HOH:O	2.03	0.58
1:F:75:GLN:NE2	1:F:266:ASP:H	2.02	0.57
1:D:305:LYS:NZ	1:D:322:GLU:OE1	2.38	0.57
1:A:75:GLN:HE22	1:A:266:ASP:H	1.52	0.57
1:F:350:PRO:O	1:F:354:VAL:HG23	2.06	0.56
1:C:362:ARG:HD3	4:C:3234:HOH:O	2.04	0.56
1:A:296:LEU:HD13	1:A:305:LYS:HE3	1.88	0.56
1:F:205:HIS:HB2	1:F:335:GLY:O	2.06	0.56
1:B:201:ARG:O	1:B:333:ASN:HB2	2.07	0.54
1:A:71:HIS:HD2	1:A:273:MET:HE2	1.72	0.54
1:B:5:ASN:HB3	4:B:3204:HOH:O	2.08	0.54
1:D:284:GLY:HA3	1:E:267:GLN:HE22	1.73	0.54
1:B:269:ARG:HD2	1:B:269:ARG:H	1.72	0.54
1:D:274:LYS:HD2	1:D:322:GLU:OE2	2.06	0.54
1:D:59:ALA:HB2	1:D:311:ILE:HB	1.90	0.53
1:F:296:LEU:HD13	1:F:305:LYS:HE3	1.91	0.53
1:F:320:ARG:HD3	4:F:3085:HOH:O	2.07	0.53
1:C:115:THR:HG22	4:C:3041:HOH:O	2.08	0.53
1:A:336:ALA:H	1:A:344:LEU:HD13	1.74	0.53
1:A:265:LEU:HD21	1:A:273:MET:HE3	1.90	0.53
1:E:59:ALA:HB2	1:E:311:ILE:HB	1.91	0.53
1:E:201:ARG:O	1:E:333:ASN:HB2	2.08	0.52
1:B:163:HIS:HD2	4:B:3207:HOH:O	1.92	0.52
1:B:119:MET:HG3	1:B:215:TRP:HB3	1.90	0.52
1:A:71:HIS:HD2	1:A:273:MET:HE3	1.73	0.52
1:C:80:ASP:O	1:C:83:GLU:HG2	2.09	0.52
1:C:267:GLN:HE22	1:E:284:GLY:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LYS:HE3	4:B:3162:HOH:O	2.08	0.52
1:C:269:ARG:N	1:C:269:ARG:HD2	2.25	0.51
1:F:75:GLN:CG	1:F:269:ARG:HD3	2.41	0.51
1:A:318:MET:HB3	1:A:329:MET:SD	2.51	0.51
1:F:269:ARG:N	1:F:269:ARG:HD2	2.26	0.50
1:C:132:ASP:O	1:C:136:ARG:HG2	2.11	0.50
1:B:48[A]:MET:HE2	4:B:3142:HOH:O	2.12	0.50
1:C:318:MET:HB3	1:C:329:MET:SD	2.51	0.50
1:D:201:ARG:O	1:D:333:ASN:HB2	2.12	0.49
1:A:71:HIS:CD2	1:A:273:MET:HE2	2.47	0.49
1:B:349:GLU:HB3	1:B:353:ARG:NH1	2.27	0.49
1:E:316:SER:HB3	1:E:331:ILE:HG23	1.95	0.49
1:B:353:ARG:NH1	4:B:3289:HOH:O	2.19	0.48
1:F:48:MET:N	4:F:3197:HOH:O	2.45	0.48
1:D:318:MET:HB3	1:D:329:MET:SD	2.53	0.48
1:F:205:HIS:CB	1:F:335:GLY:O	2.61	0.48
1:B:117:MET:HG3	1:B:118:PRO:HD2	1.95	0.48
1:B:45:PHE:CZ	1:B:224:VAL:HG12	2.49	0.48
1:D:126:THR:HG22	1:D:129:GLU:H	1.78	0.48
1:F:75:GLN:HE22	1:F:265:LEU:CA	2.27	0.48
1:A:181:LEU:O	4:A:3142:HOH:O	2.20	0.48
1:F:201:ARG:O	1:F:333:ASN:HB2	2.13	0.47
1:D:285:SER:CB	1:D:308:LEU:HD22	2.44	0.47
1:F:280:ALA:HB2	1:F:290:ASN:OD1	2.15	0.47
1:B:75:GLN:HB3	1:B:269:ARG:HD3	1.96	0.47
1:D:296:LEU:HD22	1:D:305:LYS:CD	2.43	0.47
1:D:112:ASP:OD2	1:D:114:GLU:HB3	2.15	0.47
1:D:285:SER:HB3	1:D:308:LEU:HD22	1.96	0.47
1:F:298:ARG:NH2	4:F:3178:HOH:O	2.47	0.46
1:A:58:ILE:HD13	1:A:252:ILE:HD11	1.97	0.46
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.97	0.46
1:F:260:PHE:CG	1:F:320:ARG:HD2	2.51	0.46
1:E:80:ASP:O	1:E:83:GLU:HG2	2.16	0.46
1:B:59:ALA:HB2	1:B:311:ILE:HB	1.97	0.46
1:E:75:GLN:HE22	1:E:266:ASP:N	2.13	0.46
1:F:172:HIS:CE1	1:F:176:ARG:HD3	2.51	0.46
1:D:30:PRO:HG2	1:D:324:THR:O	2.15	0.45
1:C:59:ALA:HB2	1:C:311:ILE:HB	1.98	0.45
1:B:223:PRO:HD3	1:B:228:TRP:CZ2	2.51	0.45
1:B:306:GLY:HA3	1:B:318:MET:O	2.16	0.45
1:A:59:ALA:HB2	1:A:311:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASP:OD2	1:B:114[B]:GLU:HB2	2.17	0.45
1:A:201:ARG:O	1:A:333:ASN:HB2	2.17	0.45
1:C:199:GLU:HG2	1:C:200:ALA:O	2.17	0.45
1:D:282:PHE:CE2	1:D:283:PRO:O	2.70	0.45
1:A:72:LEU:HD13	1:A:265:LEU:CD1	2.44	0.44
1:E:59:ALA:O	1:E:243:GLY:HA2	2.17	0.44
1:F:318:MET:HB3	1:F:329:MET:SD	2.57	0.44
1:E:66:ILE:HG13	1:E:241:ALA:O	2.17	0.44
1:D:282:PHE:CD2	1:D:283:PRO:O	2.71	0.44
1:A:78:THR:HG23	1:A:79:VAL:HG23	1.98	0.44
1:E:20:VAL:HG13	1:E:334:SER:HB2	2.00	0.44
1:B:260:PHE:CB	1:B:320:ARG:HD2	2.48	0.43
1:C:316:SER:HB3	1:C:331:ILE:HG23	2.00	0.43
1:B:30:PRO:HG3	1:B:324:THR:O	2.17	0.43
1:F:29:LEU:HB3	1:F:30:PRO:HD2	2.00	0.43
1:D:113:PHE:HB3	1:D:134:SER:OG	2.18	0.43
1:C:201:ARG:O	1:C:333:ASN:HB2	2.19	0.43
1:B:296:LEU:HD23	1:B:303:GLU:OE1	2.19	0.43
1:E:271:TRP:CD1	1:E:275:ASP:HB2	2.53	0.43
1:E:179:ALA:HB3	1:E:180:PRO:HD3	2.01	0.43
1:A:296:LEU:HD11	1:A:303:GLU:OE2	2.19	0.42
1:D:283:PRO:HA	1:D:284:GLY:HA2	1.86	0.42
1:F:204:MET:CA	1:F:205:HIS:HB2	2.36	0.42
1:C:48:MET:HA	1:C:49:PRO:HD2	1.88	0.42
1:B:320:ARG:HD3	4:B:3212:HOH:O	2.19	0.42
1:C:75:GLN:HE22	1:C:266:ASP:H	1.68	0.42
1:D:120:ILE:HG13	1:D:233:TRP:CG	2.55	0.42
1:A:201:ARG:HD3	1:A:229:ASP:OD2	2.20	0.42
1:F:59:ALA:HB2	1:F:311:ILE:HB	2.02	0.42
1:E:30:PRO:HG3	1:E:324:THR:O	2.20	0.42
1:B:102:ILE:HD12	1:B:144:TRP:CE2	2.56	0.41
1:E:318:MET:HB3	1:E:329:MET:SD	2.60	0.41
1:D:344:LEU:HA	1:D:344:LEU:HD12	1.87	0.41
1:E:265:LEU:HG	1:E:269:ARG:HB3	2.03	0.41
1:A:68:THR:N	1:A:273:MET:HE1	2.36	0.41
1:A:30:PRO:CG	1:A:362:ARG:HH21	2.33	0.41
1:F:51:THR:N	1:F:54:HIS:HD2	2.05	0.41
1:C:349:GLU:O	1:C:353:ARG:HG2	2.20	0.41
1:A:60:SER:O	1:A:63:LYS:HB2	2.20	0.41
1:E:5:ASN:H	1:E:5:ASN:HD22	1.67	0.41
1:D:296:LEU:HD13	1:D:303:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:ILE:HG13	1:E:196:ILE:H	1.63	0.41
1:D:179:ALA:HB3	1:D:180:PRO:HD3	2.03	0.41
1:A:268:LYS:HD3	1:F:281:PHE:CD2	2.55	0.41
1:F:260:PHE:CB	1:F:320:ARG:HD2	2.50	0.40
1:D:284:GLY:C	4:D:3069:HOH:O	2.60	0.40
1:D:80:ASP:O	1:D:83:GLU:HG2	2.21	0.40
1:E:5:ASN:N	1:E:5:ASN:HD22	2.18	0.40
1:A:280:ALA:HB2	1:A:290:ASN:OD1	2.20	0.40
1:E:2:SER:OG	1:E:5:ASN:ND2	2.55	0.40
1:D:284:GLY:HA3	1:E:267:GLN:NE2	2.35	0.40
1:C:359:LYS:HE2	1:C:359:LYS:HB3	1.89	0.40
1:C:119:MET:CG	1:C:215:TRP:HB3	2.52	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	361/363 (99%)	353 (98%)	7 (2%)	1 (0%)	46	57
1	B	357/363 (98%)	342 (96%)	12 (3%)	3 (1%)	24	27
1	C	359/363 (99%)	348 (97%)	10 (3%)	1 (0%)	46	57
1	D	347/363 (96%)	332 (96%)	14 (4%)	1 (0%)	46	57
1	E	336/363 (93%)	326 (97%)	8 (2%)	2 (1%)	30	36
1	F	326/363 (90%)	314 (96%)	12 (4%)	0	100	100
All	All	2086/2178 (96%)	2015 (97%)	63 (3%)	8 (0%)	39	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	VAL

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Mol	Chain	Res	Type
1	C	243	GLY
1	A	243	GLY
1	B	225	ASP
1	B	243	GLY
1	D	243	GLY
1	E	243	GLY
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	301/301 (100%)	292 (97%)	9 (3%)	48	65
1	B	300/301 (100%)	293 (98%)	7 (2%)	58	75
1	C	299/301 (99%)	288 (96%)	11 (4%)	41	55
1	D	291/301 (97%)	282 (97%)	9 (3%)	47	64
1	E	285/301 (95%)	277 (97%)	8 (3%)	51	68
1	F	277/301 (92%)	265 (96%)	12 (4%)	35	47
All	All	1753/1806 (97%)	1697 (97%)	56 (3%)	46	62

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	115	THR
1	A	196	ILE
1	A	201	ARG
1	A	265	LEU
1	A	307	HIS
1	A	320	ARG
1	A	344	LEU
1	A	345	LYS
1	B	92	LEU
1	B	97	GLN

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Mol	Chain	Res	Type
1	B	112	ASP
1	B	269	ARG
1	B	307	HIS
1	B	329	MET
1	B	363	SER
1	C	48	MET
1	C	112	ASP
1	C	115	THR
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
1	C	353	ARG
1	D	97	GLN
1	D	114	GLU
1	D	119	MET
1	D	122	ASP
1	D	126	THR
1	D	173	LEU
1	D	307	HIS
1	D	320	ARG
1	D	329	MET
1	E	35	SER
1	E	196	ILE
1	E	198	ARG
1	E	201	ARG
1	E	265	LEU
1	E	307	HIS
1	E	329	MET
1	E	353	ARG
1	F	6	ASN
1	F	23	VAL
1	F	48	MET
1	F	78	THR
1	F	112	ASP
1	F	114	GLU
1	F	124	SER
1	F	126	THR
1	F	136	ARG

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Mol	Chain	Res	Type
1	F	184	LYS
1	F	269	ARG
1	F	307	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

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

### 5.3.3 RNA ⓘ

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](#)

Of 32 ligands modelled in this entry, 26 are monoatomic - leaving 6 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	PHE	A	2001	-	9,12,12	0.70	0	9,15,15	0.18	0
3	PHE	B	2002	-	9,12,12	0.53	0	9,15,15	0.25	0
3	PHE	C	2003	-	9,12,12	0.59	0	9,15,15	0.26	0
3	PHE	D	2004	2	9,12,12	0.46	0	9,15,15	0.25	0
3	PHE	E	2005	-	9,12,12	0.60	0	9,15,15	0.35	0
3	PHE	F	2006	2	9,12,12	0.60	0	9,15,15	0.14	0

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	PHE	A	2001	-	-	0/4/8/8	0/1/1/1
3	PHE	B	2002	-	-	0/4/8/8	0/1/1/1
3	PHE	C	2003	-	-	0/4/8/8	0/1/1/1
3	PHE	D	2004	2	-	0/4/8/8	0/1/1/1
3	PHE	E	2005	-	-	0/4/8/8	0/1/1/1
3	PHE	F	2006	2	-	0/4/8/8	0/1/1/1

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 ⓘ

### 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%)	-0.20	4 (1%) 82 86	12, 27, 39, 54	0
1	B	359/363 (98%)	-0.31	8 (2%) 65 73	9, 17, 44, 55	0
1	C	361/363 (99%)	-0.22	8 (2%) 65 73	10, 22, 40, 46	0
1	D	350/363 (96%)	-0.27	3 (0%) 85 89	9, 19, 37, 52	0
1	E	342/363 (94%)	-0.03	9 (2%) 59 68	12, 28, 49, 59	0
1	F	330/363 (90%)	0.01	8 (2%) 62 71	16, 30, 43, 54	0
All	All	2104/2178 (96%)	-0.17	40 (1%) 70 76	9, 24, 44, 59	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	SER	5.5
1	E	45	PHE	4.6
1	E	48	MET	4.3
1	F	4	LEU	4.3
1	F	228	TRP	3.9
1	F	6	ASN	3.9
1	F	48	MET	3.2
1	B	212	ASN	3.2
1	E	343	TYR	2.9
1	C	45	PHE	2.9
1	E	226	GLY	2.9
1	C	207	ALA	2.8
1	A	2	SER	2.8
1	E	41	TYR	2.8
1	C	41	TYR	2.8
1	D	363	SER	2.7
1	F	41	TYR	2.6
1	D	119	MET	2.6
1	A	45	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	31	GLY	2.6
1	B	224	VAL	2.6
1	C	363	SER	2.5
1	C	4	LEU	2.5
1	E	203	TYR	2.5
1	E	227	VAL	2.4
1	E	228	TRP	2.4
1	C	360	ASN	2.4
1	B	208	ALA	2.3
1	F	120	ILE	2.3
1	C	208	ALA	2.3
1	F	205	HIS	2.3
1	D	118	PRO	2.2
1	B	211	GLU	2.2
1	A	41	TYR	2.1
1	A	363	SER	2.1
1	E	363	SER	2.1
1	C	47	LYS	2.1
1	F	31	GLY	2.0
1	B	362	ARG	2.0
1	B	209	ASP	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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PHE	C	2003	12/12	0.90	0.17	5.02	36,38,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PHE	E	2005	12/12	0.82	0.24	3.86	33,38,40,40	0
3	PHE	F	2006	12/12	0.82	0.23	2.48	40,42,42,42	0
3	PHE	D	2004	12/12	0.86	0.21	1.95	37,40,43,43	0
3	PHE	A	2001	12/12	0.93	0.15	1.93	31,33,33,33	0
3	PHE	B	2002	12/12	0.92	0.15	1.20	33,34,35,35	0
2	BA	A	3003	1/1	0.99	0.12	-0.15	21,21,21,21	1
2	BA	F	3025	1/1	0.99	0.07	-2.25	36,36,36,36	1
2	BA	C	3001	1/1	1.00	0.08	-2.88	27,27,27,27	1
2	BA	C	3005	1/1	0.99	0.09	-2.91	22,22,22,22	1
2	BA	F	3006	1/1	0.99	0.06	-3.10	30,30,30,30	1
2	BA	B	3010	1/1	0.87	0.43	-	49,49,49,49	1
2	BA	D	3014	1/1	0.88	0.56	-	45,45,45,45	1
2	BA	F	3021	1/1	0.84	0.16	-	42,42,42,42	1
2	BA	E	3019	1/1	0.92	0.14	-	48,48,48,48	1
2	BA	E	3012	1/1	0.92	0.14	-	44,44,44,44	1
2	BA	E	3018	1/1	0.84	0.16	-	50,50,50,50	1
2	BA	A	3020	1/1	0.78	0.12	-	46,46,46,46	1
2	BA	A	3009	1/1	0.93	0.35	-	48,48,48,48	1
2	BA	D	3017	1/1	0.93	0.09	-	57,57,57,57	1
2	BA	F	3007	1/1	0.98	0.18	-	67,67,67,67	1
2	BA	E	3024	1/1	0.97	0.06	-	44,44,44,44	1
2	BA	B	3002	1/1	0.99	0.09	-	32,32,32,32	1
2	BA	F	3016	1/1	0.93	0.06	-	48,48,48,48	1
2	BA	D	3023[B]	1/1	0.99	0.08	-	39,39,39,39	1
2	BA	F	3008	1/1	0.97	0.20	-	24,24,24,24	1
2	BA	C	3011	1/1	0.96	0.07	-	47,47,47,47	1
2	BA	D	3023[A]	1/1	0.99	0.08	-	33,33,33,33	1
2	BA	D	3022	1/1	0.92	0.11	-	53,53,53,53	1
2	BA	D	3015	1/1	0.98	0.03	-	52,52,52,52	1
2	BA	A	3004	1/1	0.91	0.08	-	62,62,62,62	1
2	BA	C	3013	1/1	0.92	0.24	-	46,46,46,46	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.