Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	2DRW
Title	:	The crystal structutre 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)

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

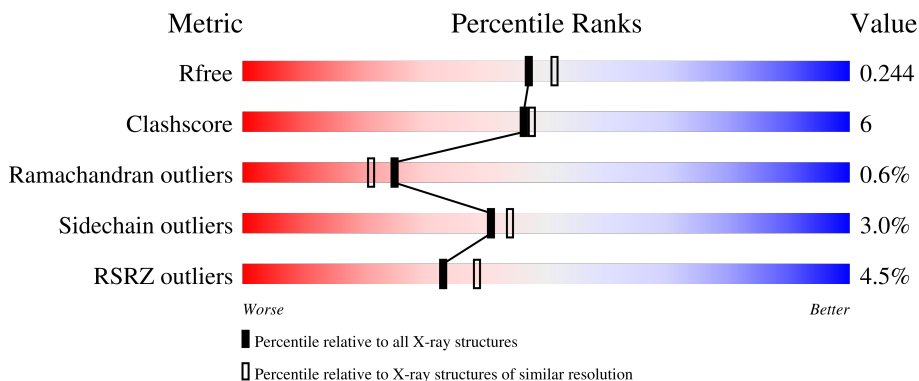|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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.
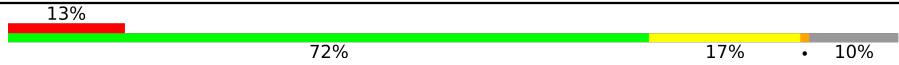
Metric	Percentile Ranks	Value
Rfree		0.244
Clashscore		6
Ramachandran outliers		0.6%
Sidechain outliers		3.0%
RSRZ outliers		4.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

◲ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	87% ... 11% ·
1	B	363	87% ... 11% ··
1	C	363	89% ... 9% ··
1	D	363	88% ... 8% · ·
1	E	363	84% ... 9% · 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	363	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 18459 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	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	A	4	Total	Ba	0	0
			4	4		
2	B	2	Total	Ba	0	0
			2	2		
2	C	3	Total	Ba	0	0
			3	3		
2	D	5	Total	Ba	0	0
			5	5		
2	E	3	Total	Ba	0	0
			3	3		
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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

- Molecule 1: D-Amino acid amidase

- Molecule 1: D-Amino acid amidase

- Molecule 1: D-Amino acid amidase

L296 E303 E322 E323 T324 M329 N333 S334 G335 F339 L344 R362 S363

• Molecule 1: D-Amino acid amidase

Chain E:

5%

84%   9%   • 5%

MET S2 N6 V16 A17 R18 G19 V20 S24 Y41 K44 PHE N46 K47 M48 P49 M50 T51 H54 L55 A59 Q75 D80 E83 Q97 D112 R136 H137 A179 P180 P195 I196 E197 R198 R201 G202 Y203 A206 ALA ALA ASP ASP GLU

ASN PRO GLN TRP VAL SER GLY ALA GLY ASP P223 V224 D225 G226 V227 W228 D229 G243 L265 D266 R269 A280 G284 N290 H307 I311 P312 S316 I317 M318 M329 L330 I331 Q332 N333 Y343 R353 S363

• Molecule 1: D-Amino acid amidase

Chain F:

13%

72%   17%   • 10%

MET SER ASP LEU ASN ASN A7 I11 D14 H15 G19 V20 V21 G22 V23 S24 L25 L29 P30 G31 S35 L36 Y37 G40 Y41 A42 D43 K44 PHE ASN LYS M48 P49 M50 T51 H54 L55 S60 V74 Q75 V79 D80 E83 P84 I85 L103 T115

S116 M117 P118 M119 I120 K123 S124 W125 T126 Y149 F178 A179 P180 L181 K184 W187 V188 G189 T193 I196 R201 M204 H205 ALA ALA ALA ASP ASP GLU ASN PRO GLN TRP ASP VAL SER GLY ALA GLY ASP PRO VAL ASP GLY VAL W228 E232 W233 N240

G243 D244 M245 T248 P249 R250 D251 K254 F255 F260 L265 D266 Q267 K268 R269 L270 M273 K274 A280 F281 G284 N290 R298 E303 G306 H307 I311 P312 G319 R320 T324 G325 A326 M329 L330 N333 S334 G335 A336 F339 F342

Y343 L344 K345 G346 R353 I358 LYS ASN SER ARG SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18459	wwPDB-VP
Average B, all atoms (Å^2)	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

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

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 (201) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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: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:HD12	1:F:273:MET:HE3	1.63	0.80
1:A:75:GLN:NE2	1:A:266:ASP:H	1.80	0.79
1:F:265:LEU:HD11	1:F:273:MET:CE	2.12	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:57:ARG:H	1:A:314:HIS:HD2	1.37	0.72
1:A:196:ILE:HD12	1:A:196:ILE:H	1.54	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:E:75:GLN:HE22	1:E:265:LEU:HA	1.56	0.69
1:F:75:GLN:NE2	1:F:266:ASP:H	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLN:NE2	1:C:266:ASP:H	1.92	0.68
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:B:30:PRO:HG3	1:B:324:THR:O	1.97	0.64
1:E:75:GLN:HE22	1:E:266:ASP:H	1.43	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:B:274:LYS:O	1:B:305:LYS:HE2	2.05	0.56
1:C:75:GLN:HG2	1:C:269:ARG:HD3	1.88	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:214:GLN:HG2	1:B:337:GLY:O	2.13	0.49
1:F:267:GLN:NE2	3:F:3171:HOH:O	2.44	0.49
1:D:274:LYS:HD2	1:D:322:GLU:OE2	2.13	0.48
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: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:D:339:PHE:HA	1:D:344:LEU:HD23	1.94	0.47
1:E:46:ASN:N	1:E:47:LYS:CA	2.77	0.47
1:A:265:LEU:HG	1:A:269:ARG:HB3	1.96	0.47
1:D:113:PHE:HB3	1:D:134:SER:OG	2.14	0.47
1:F:306:GLY:HA3	1:F:319:GLY:HA2	1.96	0.47
1:C:318:MET:HB3	1:C:329:MET:SD	2.54	0.47
1:E:75:GLN:HE22	1:E:266:ASP:N	2.10	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	1:A:196:ILE:CD1	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:E:280:ALA:HB2	1:E:290:ASN:OD1	2.17	0.44
1:F:311:ILE:O	1:F:312:PRO:C	2.55	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:74:VAL:HA	1:D:79:VAL:O	2.19	0.43
1:D:201:ARG:O	1:D:333:ASN:HB2	2.18	0.43
1:F:249:PRO:HB3	1:F:329:MET:O	2.18	0.43
1:C:126:THR:HG21	3:C:3314:HOH:O	2.19	0.42
1:C:269:ARG:HD2	1:C:269:ARG:N	2.34	0.42
1:C:344:LEU:HD12	1:C:344:LEU:HA	1.84	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HB3	1:A:134:SER:OG	2.19	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
1:F:260:PHE:CB	1:F:320:ARG:HD2	2.49	0.42
1:E:196:ILE:H	1:E:196:ILE:HG13	1.61	0.42
1:F:75:GLN:HE22	1:F:266:ASP:H	1.64	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:136:ARG:NH2	3:A:3087:HOH:O	2.53	0.42
1:A:353:ARG:HG2	3:A:3370:HOH:O	2.19	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:162:ALA:HA	1:A:167:LYS:O	2.20	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:B:274:LYS:HB2	1:B:305:LYS:HD2	2.02	0.41
1:F:21:VAL:HG23	1:F:205:HIS:HE1	1.84	0.41
1:A:15:HIS:NE2	1:A:20:VAL:HG21	2.36	0.41
1:A:68:THR:HA	1:A:273:MET:HE1	2.03	0.41
1:C:51:THR:H	1:C:54:HIS:CD2	2.19	0.41
1:D:199:GLU:HG2	1:D:200:ALA:O	2.21	0.41
1:D:283:PRO:HA	1:D:284:GLY:HA2	1.78	0.41
1:F:204:MET:HA	1:F:205:HIS:CB	2.43	0.41
1:B:196:ILE:O	1:B:196:ILE:HG13	2.21	0.40
1:B:296:LEU:HD23	1:B:303:GLU:OE1	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:B:2:SER:HA	1:C:226:GLY:HA3	2.03	0.40
1:F:126:THR:HG21	3:F:3075:HOH:O	2.21	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	Interatomic distance (Å)	Clash overlap (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%)	41	41
1	B	362/363 (100%)	344 (95%)	14 (4%)	4 (1%)	14	9
1	C	354/363 (98%)	343 (97%)	10 (3%)	1 (0%)	41	41
1	D	346/363 (95%)	335 (97%)	10 (3%)	1 (0%)	41	41
1	E	339/363 (93%)	329 (97%)	7 (2%)	3 (1%)	17	12
1	F	321/363 (88%)	309 (96%)	10 (3%)	2 (1%)	25	21
All	All	2082/2178 (96%)	2008 (96%)	62 (3%)	12 (1%)	25	21

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%)	41	44
1	B	302/301 (100%)	291 (96%)	11 (4%)	35	36
1	C	298/301 (99%)	288 (97%)	10 (3%)	37	39
1	D	290/301 (96%)	285 (98%)	5 (2%)	60	67
1	E	288/301 (96%)	281 (98%)	7 (2%)	49	53
1	F	272/301 (90%)	261 (96%)	11 (4%)	31	32
All	All	1750/1806 (97%)	1697 (97%)	53 (3%)	41	44

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	329	MET
1	C	344	LEU
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

Sometimes 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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 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 monosaccharides 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.

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, 95th 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^2)	Q<0.9
1	A	362/363 (99%)	-0.28	3 (0%)	86	88	11, 23, 36, 45	0
1	B	362/363 (99%)	-0.23	13 (3%)	42	49	10, 17, 46, 57	0
1	C	358/363 (98%)	-0.27	7 (1%)	65	69	10, 20, 40, 52	0
1	D	350/363 (96%)	-0.30	5 (1%)	75	78	9, 18, 36, 53	0
1	E	345/363 (95%)	0.19	18 (5%)	27	32	15, 31, 53, 64	0
1	F	327/363 (90%)	0.76	48 (14%)	2	3	15, 37, 56, 63	0
All	All	2104/2178 (96%)	-0.03	94 (4%)	33	38	9, 24, 50, 64	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	VAL	7.4
1	F	41	TYR	6.2
1	F	31	GLY	5.6
1	F	40	GLY	5.6
1	B	2	SER	5.6
1	E	227	VAL	5.5
1	F	37	TYR	5.3
1	C	363	SER	5.0
1	E	225	ASP	5.0
1	E	48	MET	5.0
1	E	206	ALA	4.8
1	F	120	ILE	4.5
1	B	363	SER	4.4
1	E	41	TYR	4.3
1	F	196	ILE	4.3
1	B	208	ALA	4.3
1	F	22	GLY	4.3
1	B	212	ASN	4.1
1	F	21	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	11	ILE	4.1
1	D	363	SER	4.0
1	F	204	MET	3.8
1	F	228	TRP	3.6
1	F	344	LEU	3.6
1	C	360	ASN	3.4
1	B	31	GLY	3.4
1	F	193	THR	3.4
1	C	45	PHE	3.4
1	F	20	VAL	3.4
1	F	189	GLY	3.3
1	F	115	THR	3.3
1	C	3	ASP	3.2
1	B	207	ALA	3.1
1	F	48	MET	3.1
1	E	51	THR	3.1
1	F	233	TRP	3.0
1	F	343	TYR	3.0
1	F	205	HIS	3.0
1	F	339	PHE	2.9
1	F	181	LEU	2.9
1	E	46	ASN	2.9
1	F	249	PRO	2.9
1	F	29	LEU	2.9
1	F	30	PRO	2.9
1	F	49	PRO	2.8
1	C	5	ASN	2.8
1	E	224	VAL	2.8
1	B	3	ASP	2.8
1	B	209	ASP	2.7
1	E	44	LYS	2.7
1	B	362	ARG	2.7
1	D	115	THR	2.6
1	F	25	LEU	2.6
1	F	179	ALA	2.6
1	F	346	GLY	2.6
1	F	326	ALA	2.6
1	E	198	ARG	2.5
1	E	228	TRP	2.5
1	A	224	VAL	2.5
1	F	333	ASN	2.5
1	D	207	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	187	TRP	2.4
1	F	353	ARG	2.4
1	F	312	PRO	2.4
1	B	45	PHE	2.4
1	F	35	SER	2.4
1	C	41	TYR	2.4
1	E	203	TYR	2.4
1	E	18	ARG	2.3
1	F	15	HIS	2.3
1	F	44	LYS	2.3
1	B	216[A]	ASP	2.3
1	A	234	PHE	2.3
1	F	14	ASP	2.3
1	F	255	PHE	2.3
1	F	43	ASP	2.3
1	F	19	GLY	2.3
1	F	342	PHE	2.2
1	E	49	PRO	2.2
1	E	226	GLY	2.2
1	B	220	ALA	2.2
1	C	361	SER	2.2
1	E	55	LEU	2.2
1	E	343	TYR	2.2
1	F	23	VAL	2.2
1	A	363	SER	2.1
1	D	2	SER	2.1
1	F	55	LEU	2.1
1	F	178	PHE	2.1
1	F	36	LEU	2.1
1	F	42	ALA	2.1
1	E	47	LYS	2.0
1	D	362	ARG	2.0
1	F	248	THR	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 monosaccharides 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, 95th 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($Å^2$)	Q<0.9
2	BA	E	3019	1/1	0.75	0.09	56,56,56,56	1
2	BA	F	3021	1/1	0.78	0.10	76,76,76,76	1
2	BA	D	3014	1/1	0.81	0.18	45,45,45,45	1
2	BA	D	3022	1/1	0.81	0.12	55,55,55,55	1
2	BA	A	3020	1/1	0.88	0.06	52,52,52,52	1
2	BA	B	3010	1/1	0.88	0.22	46,46,46,46	1
2	BA	A	3009	1/1	0.90	0.30	47,47,47,47	1
2	BA	E	3018	1/1	0.92	0.06	47,47,47,47	1
2	BA	F	3008	1/1	0.93	0.23	44,44,44,44	1
2	BA	B	3002	1/1	0.93	0.10	43,43,43,43	1
2	BA	C	3011	1/1	0.94	0.05	46,46,46,46	1
2	BA	E	3012	1/1	0.94	0.08	49,49,49,49	1
2	BA	F	3023	1/1	0.94	0.05	70,70,70,70	1
2	BA	D	3017	1/1	0.95	0.07	59,59,59,59	1
2	BA	F	3016	1/1	0.95	0.07	72,72,72,72	1
2	BA	D	3015	1/1	0.96	0.05	45,45,45,45	1
2	BA	A	3004	1/1	0.98	0.06	34,34,34,34	1
2	BA	F	3006	1/1	0.98	0.06	43,43,43,43	1
2	BA	A	3003	1/1	0.98	0.05	37,37,37,37	1
2	BA	D	3013	1/1	0.99	0.11	44,44,44,44	1
2	BA	C	3005	1/1	0.99	0.06	20,20,20,20	1
2	BA	C	3001	1/1	0.99	0.06	34,34,34,34	1
2	BA	F	3007	1/1	0.99	0.10	52,52,52,52	1

6.5 Other polymers (i)

There are no such residues in this entry.