Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 10:51 AM EST

PDB ID	:	3N7Z
Title	:	Crystal structure of acetyltransferase from Bacillus anthracis
Authors	:	Chang, C.; Wu, R.; Gornicki, P.; Zhang, R.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2010-05-27
Resolution	:	2.75 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

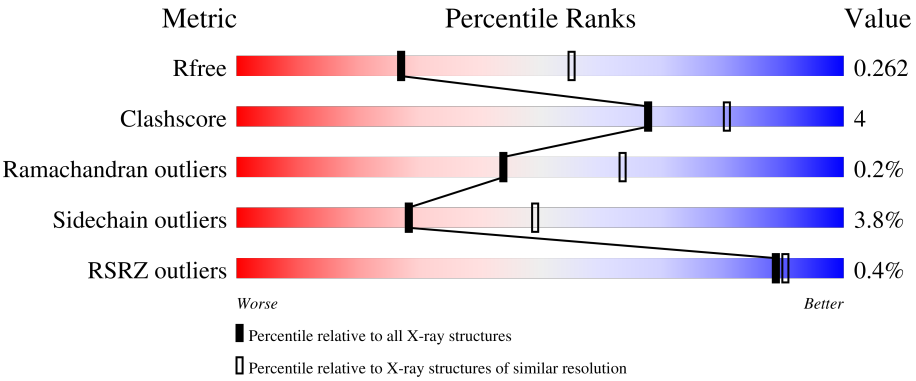
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	388	85% 13%
1	B	388	86% 12%
1	C	388	% 86% 12%
1	D	388	89% 9%
1	E	388	% 84% 12%

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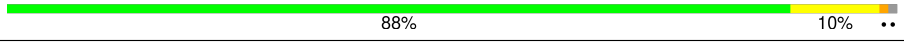
Mol	Chain	Length	Quality of chain
1	F	388	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19022 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 Acetyltransferase, GNAT family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	Se	0	0	0
			3152	2037	522	577	3	13			
1	B	384	Total	C	N	O	S	Se	0	0	0
			3187	2056	526	589	3	13			
1	C	381	Total	C	N	O	S	Se	0	0	0
			3135	2028	516	575	3	13			
1	D	383	Total	C	N	O	S	Se	0	0	0
			3164	2046	522	580	3	13			
1	E	379	Total	C	N	O	S	Se	0	0	0
			3128	2026	516	570	3	13			
1	F	383	Total	C	N	O	S	Se	0	0	0
			3158	2040	521	581	3	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	-	expression tag	UNP Q6HXD7
A	4	ASN	-	expression tag	UNP Q6HXD7
A	5	ALA	-	expression tag	UNP Q6HXD7
B	3	SER	-	expression tag	UNP Q6HXD7
B	4	ASN	-	expression tag	UNP Q6HXD7
B	5	ALA	-	expression tag	UNP Q6HXD7
C	3	SER	-	expression tag	UNP Q6HXD7
C	4	ASN	-	expression tag	UNP Q6HXD7
C	5	ALA	-	expression tag	UNP Q6HXD7
D	3	SER	-	expression tag	UNP Q6HXD7
D	4	ASN	-	expression tag	UNP Q6HXD7
D	5	ALA	-	expression tag	UNP Q6HXD7
E	3	SER	-	expression tag	UNP Q6HXD7
E	4	ASN	-	expression tag	UNP Q6HXD7
E	5	ALA	-	expression tag	UNP Q6HXD7
F	3	SER	-	expression tag	UNP Q6HXD7
F	4	ASN	-	expression tag	UNP Q6HXD7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	5	ALA	-	expression tag	UNP Q6HXD7

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

- Molecule 3 is water.

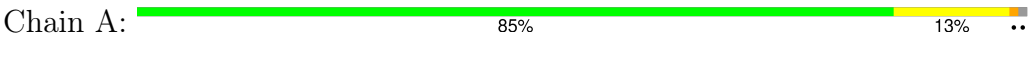
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	16	Total O 16 16	0	0
3	C	17	Total O 17 17	0	0
3	D	15	Total O 15 15	0	0
3	E	12	Total O 12 12	0	0
3	F	13	Total O 13 13	0	0

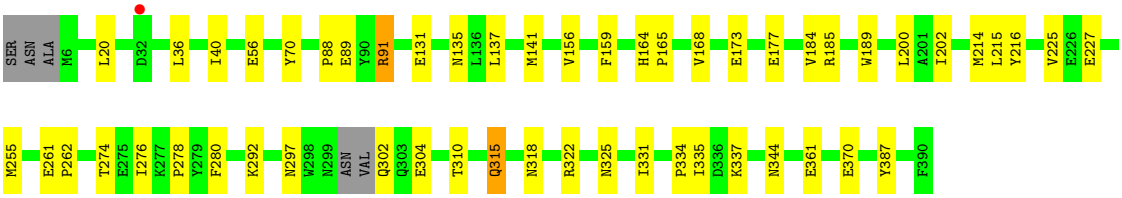
3 Residue-property plots (i)

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: Acetyltransferase, GNAT family

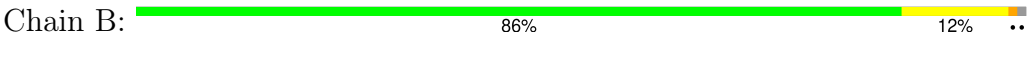
Chain A:

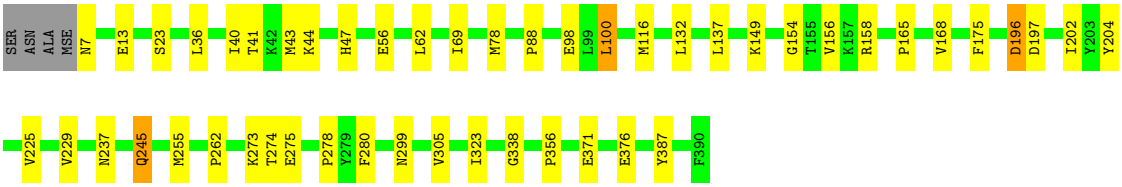




• Molecule 1: Acetyltransferase, GNAT family

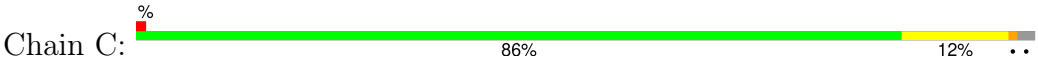
Chain B:

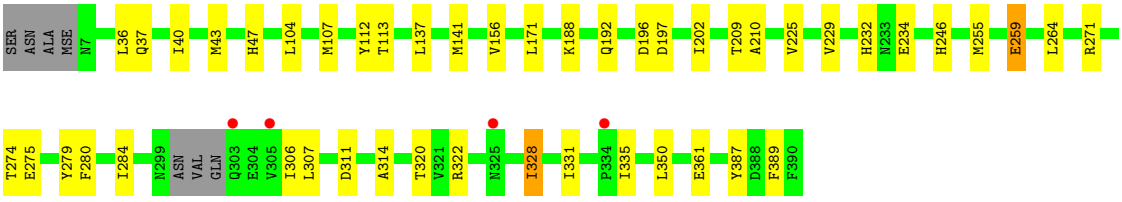




• Molecule 1: Acetyltransferase, GNAT family

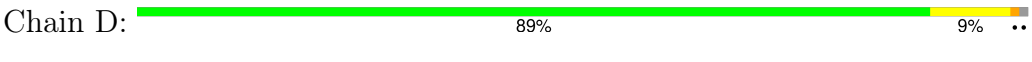
Chain C:





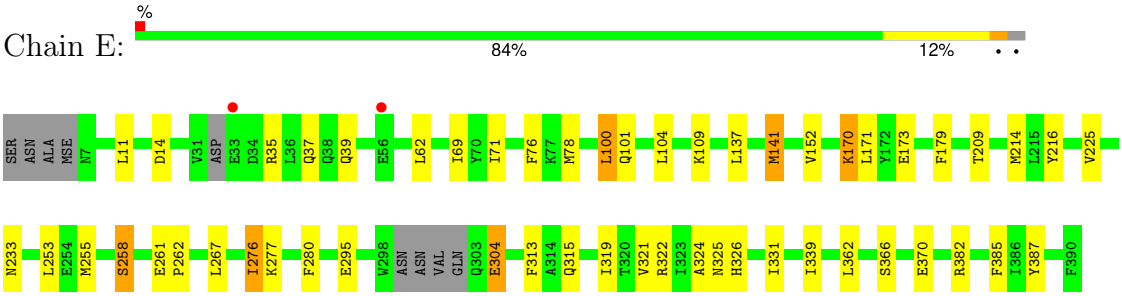
• Molecule 1: Acetyltransferase, GNAT family

Chain D:



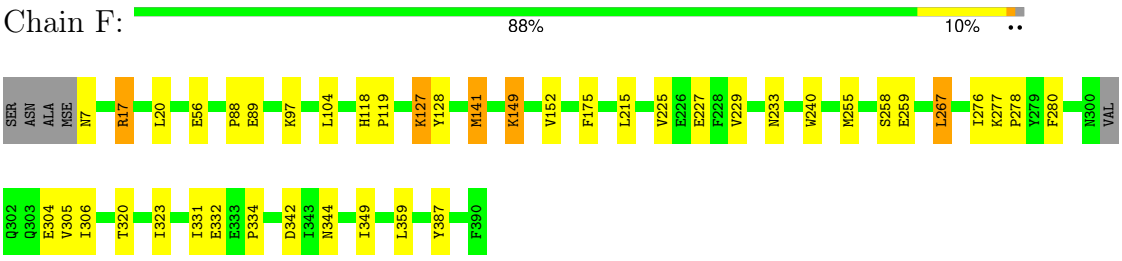
• Molecule 1: Acetyltransferase, GNAT family

Chain E:



• Molecule 1: Acetyltransferase, GNAT family

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.43Å 176.86Å 109.97Å 90.00° 105.73° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 50.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.75) 99.4 (50.00-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.242 0.219 , 0.262	Depositor DCC
R_{free} test set	3782 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 14.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19022	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: NA

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	0/3212	0.59	1/4319 (0.0%)
1	B	0.51	0/3249	0.61	0/4369
1	C	0.49	0/3195	0.59	0/4297
1	D	0.50	0/3225	0.61	0/4335
1	E	0.50	0/3188	0.61	0/4284
1	F	0.50	0/3219	0.60	0/4328
All	All	0.50	0/19288	0.60	1/25932 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	334	PRO	N-CA-CB	5.70	110.14	103.30

There are no chirality outliers.

There are no planarity outliers.

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	3152	0	3085	26	0
1	B	3187	0	3137	32	0
1	C	3135	0	3074	28	0
1	D	3164	0	3112	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3128	0	3079	21	0
1	F	3158	0	3091	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	19	0	0	0	0
3	B	16	0	0	0	0
3	C	17	0	0	1	0
3	D	15	0	0	0	0
3	E	12	0	0	0	0
3	F	13	0	0	0	0
All	All	19022	0	18578	132	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 4.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:MSE:HE2	1:B:116:MSE:CE	1.95	0.97
1:F:141:MSE:HE3	1:F:267:LEU:HD21	1.46	0.96
1:B:78:MSE:HE2	1:B:116:MSE:HE2	1.51	0.90
1:A:131:GLU:HG2	1:A:344:ASN:HB3	1.55	0.89
1:A:322:ARG:HB2	1:A:331:ILE:HD11	1.61	0.81
1:C:259:GLU:HG3	3:C:392:HOH:O	1.82	0.78
1:B:13:GLU:HG2	1:B:44:LYS:HE3	1.69	0.75
1:D:255:MSE:HE1	1:D:263:LEU:HD23	1.70	0.72
1:D:141:MSE:HE1	1:D:255:MSE:HE2	1.71	0.72
1:B:69:ILE:HG21	1:B:116:MSE:HE2	1.75	0.68
1:B:78:MSE:HE2	1:B:116:MSE:HE3	1.74	0.68
1:D:20:LEU:HD13	1:D:36:LEU:HD11	1.76	0.67
1:F:304:GLU:OE2	1:F:306:ILE:HD11	1.97	0.65
1:B:225:VAL:HB	1:B:255:MSE:HG2	1.80	0.62
1:D:52:ILE:HD12	1:D:95:TYR:HB3	1.81	0.62
1:C:137:LEU:HD11	1:C:274:THR:HG23	1.83	0.61
1:A:88:PRO:HB3	1:B:245:GLN:HB3	1.83	0.61
1:B:69:ILE:HG21	1:B:116:MSE:CE	2.31	0.60
1:B:43:MSE:HA	1:B:47:HIS:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:LYS:HG3	1:F:240:TRP:CD1	2.38	0.58
1:A:88:PRO:O	1:B:245:GLN:HG2	2.02	0.58
1:C:322:ARG:HB2	1:C:331:ILE:HD11	1.84	0.58
1:E:225:VAL:HB	1:E:255:MSE:HG2	1.85	0.58
1:D:330:ILE:H	1:D:330:ILE:HD12	1.69	0.57
1:F:149:LYS:HG3	1:F:240:TRP:HD1	1.71	0.55
1:E:141:MSE:HG3	1:E:253:LEU:HD23	1.88	0.55
1:A:315:GLN:HA	1:A:318:ASN:HD22	1.71	0.55
1:E:325:ASN:O	1:E:326:HIS:HB2	2.08	0.54
1:A:89:GLU:OE2	1:B:158:ARG:NH1	2.39	0.54
1:E:101:GLN:HB2	1:E:313:PHE:CZ	2.42	0.54
1:A:335:ILE:HG22	1:A:337:LYS:H	1.73	0.54
1:E:141:MSE:CG	1:E:253:LEU:HD23	2.38	0.54
1:A:173:GLU:O	1:A:177:GLU:HG3	2.08	0.53
1:A:185:ARG:HG2	1:A:189:TRP:CD1	2.44	0.53
1:B:88:PRO:HG2	1:C:246:HIS:NE2	2.23	0.53
1:C:306:ILE:HD11	1:C:322:ARG:HH11	1.73	0.52
1:F:225:VAL:HB	1:F:255:MSE:HG2	1.90	0.52
1:B:262:PRO:HB2	1:D:362:LEU:HD21	1.90	0.52
1:B:154:GLY:HA3	1:B:204:TYR:O	2.10	0.52
1:D:61:LYS:NZ	1:D:83:GLY:O	2.40	0.52
1:A:262:PRO:HB2	1:E:362:LEU:HD21	1.93	0.50
1:B:36:LEU:O	1:B:40:ILE:HG12	2.12	0.49
1:B:62:LEU:C	1:B:62:LEU:HD23	2.33	0.49
1:D:304:GLU:HB3	1:D:324:ALA:HB2	1.93	0.49
1:F:342:ASP:HB3	1:F:344:ASN:H	1.77	0.48
1:C:171:LEU:HD11	1:C:210:ALA:HB1	1.94	0.48
1:F:215:LEU:HB2	1:F:227:GLU:HB2	1.95	0.48
1:E:179:PHE:O	1:E:382:ARG:HD2	2.13	0.48
1:D:158:ARG:NH1	1:F:89:GLU:OE2	2.47	0.48
1:A:137:LEU:HD21	1:A:274:THR:HG23	1.96	0.47
1:B:165:PRO:O	1:B:168:VAL:HG12	2.14	0.47
1:C:137:LEU:HD11	1:C:274:THR:CG2	2.44	0.47
1:C:43:MSE:HA	1:C:47:HIS:HB2	1.97	0.47
1:D:146:LEU:HD21	1:D:253:LEU:HD22	1.96	0.47
1:E:319:ILE:HD12	1:E:321:VAL:HG23	1.95	0.47
1:B:356:PRO:HG2	1:B:376:GLU:HA	1.97	0.46
1:F:276:ILE:O	1:F:276:ILE:HG13	2.15	0.46
1:A:36:LEU:O	1:A:40:ILE:HG12	2.15	0.46
1:C:306:ILE:HD11	1:C:322:ARG:NH1	2.30	0.46
1:D:107:MSE:HA	1:D:112:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ILE:HD12	1:D:330:ILE:N	2.30	0.46
1:A:165:PRO:O	1:A:168:VAL:HG12	2.15	0.46
1:D:275:GLU:HG2	1:D:277:LYS:HG2	1.97	0.46
1:D:71:ILE:HD12	1:D:76:PHE:CD2	2.52	0.45
1:A:70:TYR:CE2	1:A:184:VAL:HG22	2.52	0.45
1:B:156:VAL:HA	1:B:202:ILE:O	2.16	0.45
1:C:232:HIS:CE1	1:C:234:GLU:HB3	2.52	0.45
1:A:159:PHE:HB2	1:A:200:LEU:HB3	1.97	0.45
1:C:141:MSE:HE1	1:C:255:MSE:CE	2.46	0.45
1:C:196:ASP:HB3	1:C:197:ASP:H	1.45	0.45
1:E:304:GLU:HB2	1:E:324:ALA:HB2	1.99	0.45
1:E:261:GLU:HA	1:E:262:PRO:HD3	1.83	0.44
1:E:339:ILE:HA	1:E:366:SER:O	2.17	0.44
1:A:214:MSE:HE2	1:A:216:TYR:CD1	2.52	0.44
1:C:225:VAL:HB	1:C:255:MSE:HG2	2.00	0.44
1:D:208:GLN:O	1:D:208:GLN:HG3	2.18	0.44
1:B:305:VAL:HB	1:B:323:ILE:HB	1.99	0.44
1:E:170:LYS:NZ	1:E:173:GLU:OE1	2.49	0.44
1:A:141:MSE:SE	1:A:255:MSE:HE2	2.68	0.43
1:A:225:VAL:HB	1:A:255:MSE:HG2	2.00	0.43
1:B:137:LEU:HD11	1:B:274:THR:CG2	2.48	0.43
1:E:137:LEU:HD12	1:E:276:ILE:HG23	2.00	0.43
1:F:17:ARG:H	1:F:17:ARG:HG2	1.56	0.43
1:F:349:ILE:HD11	1:F:359:LEU:HD12	1.99	0.43
1:B:88:PRO:HG2	1:C:246:HIS:CE1	2.53	0.43
1:C:229:VAL:HG12	1:C:229:VAL:O	2.19	0.43
1:F:175:PHE:CG	1:F:229:VAL:HG13	2.54	0.43
1:F:305:VAL:HB	1:F:323:ILE:HB	1.99	0.43
1:F:320:THR:HG22	1:F:331:ILE:HD12	2.00	0.43
1:A:261:GLU:HA	1:A:262:PRO:HD3	1.68	0.43
1:B:278:PRO:HB2	1:D:271:ARG:HG2	2.01	0.43
1:D:255:MSE:HE1	1:D:263:LEU:CD2	2.44	0.43
1:A:164:HIS:HA	1:A:165:PRO:HD3	1.89	0.42
1:C:141:MSE:SE	1:C:255:MSE:HE2	2.69	0.42
1:C:107:MSE:HA	1:C:112:TYR:HD2	1.85	0.42
1:D:101:GLN:HB2	1:D:313:PHE:CZ	2.55	0.42
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.93	0.42
1:B:175:PHE:CG	1:B:229:VAL:HG13	2.53	0.42
1:A:361:GLU:O	1:E:233:ASN:HB2	2.20	0.42
1:B:338:GLY:HA2	1:B:371:GLU:OE2	2.18	0.42
1:C:271:ARG:HG2	1:F:278:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:LYS:HG3	1:F:128:TYR:CE1	2.55	0.42
1:A:215:LEU:HB2	1:A:227:GLU:HB2	2.02	0.41
1:C:307:LEU:O	1:C:320:THR:HA	2.21	0.41
1:C:311:ASP:OD2	1:C:314:ALA:HB3	2.21	0.41
1:B:100:LEU:HD12	1:B:100:LEU:HA	1.82	0.41
1:E:62:LEU:HD12	1:E:100:LEU:HD12	2.02	0.41
1:B:132:LEU:HD11	1:D:270:PRO:HG2	2.02	0.41
1:C:36:LEU:O	1:C:40:ILE:HG12	2.20	0.41
1:C:284:ILE:CD1	1:C:350:LEU:HD12	2.49	0.41
1:F:118:HIS:HA	1:F:119:PRO:HD3	1.93	0.41
1:B:196:ASP:HB3	1:B:197:ASP:H	1.45	0.41
1:A:91:ARG:HD2	1:B:245:GLN:HG3	2.02	0.41
1:D:246:HIS:NE2	1:F:88:PRO:HG2	2.36	0.41
1:E:322:ARG:HD3	1:E:331:ILE:HD11	2.03	0.41
1:B:7:ASN:ND2	1:B:98:GLU:OE1	2.49	0.41
1:C:328:ILE:H	1:C:328:ILE:HG13	1.77	0.41
1:F:127:LYS:HD3	1:F:128:TYR:CZ	2.56	0.41
1:A:156:VAL:HA	1:A:202:ILE:O	2.21	0.41
1:C:156:VAL:HA	1:C:202:ILE:O	2.21	0.41
1:C:361:GLU:O	1:F:233:ASN:HB2	2.22	0.40
1:E:214:MSE:HE2	1:E:216:TYR:CD1	2.57	0.40
1:E:258:SER:HA	1:E:385:PHE:CE1	2.56	0.40
1:A:135:ASN:OD1	1:A:278:PRO:HA	2.21	0.40
1:B:273:LYS:HD2	1:D:275:GLU:OE1	2.20	0.40
1:C:188:LYS:HE2	1:C:192:GLN:OE1	2.21	0.40
1:E:71:ILE:HD12	1:E:76:PHE:CD2	2.56	0.40
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.98	0.40
1:B:149:LYS:HD2	1:B:237:ASN:OD1	2.20	0.40
1:C:279:TYR:OH	1:C:389:PHE:HB2	2.22	0.40
1:E:69:ILE:HG12	1:E:78:MSE:HB2	2.03	0.40
1:E:109:LYS:HE3	1:E:109:LYS:HB3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	379/388 (98%)	367 (97%)	12 (3%)	0	100	100
1	B	382/388 (98%)	366 (96%)	15 (4%)	1 (0%)	37	55
1	C	377/388 (97%)	354 (94%)	22 (6%)	1 (0%)	37	55
1	D	379/388 (98%)	362 (96%)	16 (4%)	1 (0%)	37	55
1	E	373/388 (96%)	356 (95%)	17 (5%)	0	100	100
1	F	379/388 (98%)	360 (95%)	18 (5%)	1 (0%)	37	55
All	All	2269/2328 (98%)	2165 (95%)	100 (4%)	4 (0%)	44	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	GLU
1	D	13	GLU
1	F	334	PRO
1	B	299	ASN

5.3.2 Protein sidechains (i)

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	336/338 (99%)	323 (96%)	13 (4%)	27	48
1	B	346/338 (102%)	337 (97%)	9 (3%)	41	63
1	C	335/338 (99%)	326 (97%)	9 (3%)	40	61
1	D	340/338 (101%)	331 (97%)	9 (3%)	41	63
1	E	335/338 (99%)	313 (93%)	22 (7%)	14	25
1	F	338/338 (100%)	322 (95%)	16 (5%)	22	40
All	All	2030/2028 (100%)	1952 (96%)	78 (4%)	28	49

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	91	ARG
1	A	276	ILE
1	A	280	PHE
1	A	292	LYS
1	A	297	ASN
1	A	302	GLN
1	A	304	GLU
1	A	310	THR
1	A	315	GLN
1	A	325	ASN
1	A	370	GLU
1	A	387	TYR
1	B	23	SER
1	B	41	THR
1	B	56	GLU
1	B	100	LEU
1	B	196	ASP
1	B	245	GLN
1	B	275	GLU
1	B	280	PHE
1	B	387	TYR
1	C	37	GLN
1	C	113	THR
1	C	209	THR
1	C	264	LEU
1	C	275	GLU
1	C	280	PHE
1	C	328	ILE
1	C	335	ILE
1	C	387	TYR
1	D	56	GLU
1	D	219	GLU
1	D	277	LYS
1	D	280	PHE
1	D	289	GLN
1	D	304	GLU
1	D	321	VAL
1	D	328	ILE
1	D	387	TYR
1	E	11	LEU
1	E	14	ASP
1	E	35	ARG

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Mol	Chain	Res	Type
1	E	37	GLN
1	E	39	GLN
1	E	100	LEU
1	E	104	LEU
1	E	141	MSE
1	E	152	VAL
1	E	170	LYS
1	E	171	LEU
1	E	209	THR
1	E	258	SER
1	E	267	LEU
1	E	276	ILE
1	E	277	LYS
1	E	280	PHE
1	E	295	GLU
1	E	304	GLU
1	E	315	GLN
1	E	370	GLU
1	E	387	TYR
1	F	7	ASN
1	F	17	ARG
1	F	20	LEU
1	F	56	GLU
1	F	104	LEU
1	F	127	LYS
1	F	141	MSE
1	F	149	LYS
1	F	152	VAL
1	F	258	SER
1	F	259	GLU
1	F	267	LEU
1	F	277	LYS
1	F	280	PHE
1	F	332	GLU
1	F	387	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	245	GLN
1	A	260	ASN

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Mol	Chain	Res	Type
1	A	318	ASN
1	B	68	HIS
1	C	37	GLN
1	D	192	GLN
1	F	220	ASN
1	F	260	ASN
1	F	326	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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 (i)

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^{th} 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	369/388 (95%)	-0.30	1 (0%) 90 91	3, 30, 38, 48	0
1	B	371/388 (95%)	-0.41	0 100 100	11, 27, 39, 44	0
1	C	368/388 (94%)	-0.37	4 (1%) 77 80	3, 28, 38, 46	0
1	D	370/388 (95%)	-0.35	1 (0%) 90 91	4, 28, 39, 47	0
1	E	366/388 (94%)	-0.44	2 (0%) 87 89	4, 28, 37, 49	0
1	F	370/388 (95%)	-0.41	0 100 100	10, 28, 37, 46	0
All	All	2214/2328 (95%)	-0.38	8 (0%) 89 90	3, 28, 38, 49	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	56	GLU	3.2
1	C	325	ASN	3.1
1	D	31	VAL	2.5
1	C	305	VAL	2.4
1	E	33	GLU	2.3
1	C	303	GLN	2.3
1	C	334	PRO	2.1
1	A	32	ASP	2.1

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, 95^{th} 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	NA	B	401	1/1	0.66	0.40	49,49,49,49	0
2	NA	C	401	1/1	0.76	0.32	48,48,48,48	0
2	NA	D	401	1/1	0.80	0.34	43,43,43,43	0
2	NA	E	401	1/1	0.85	0.36	39,39,39,39	0
2	NA	F	401	1/1	0.88	0.33	40,40,40,40	0
2	NA	A	401	1/1	0.91	0.33	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.