



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:59 AM UTC

PDB ID : 7YC4 / pdb_00007yc4
Title : Acetylsterase (LgEstI) F207A
Authors : Do, H.; Lee, J.H.
Deposited on : 2022-06-30
Resolution : 2.10 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

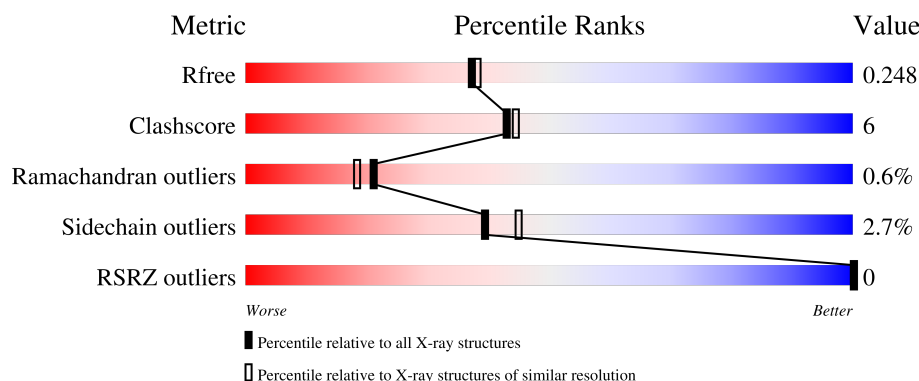
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

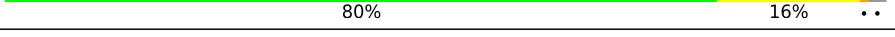
The reported resolution of this entry is 2.10 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	320	
1	B	320	
1	C	320	
1	D	320	
1	E	320	

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Mol	Chain	Length	Quality of chain
1	F	320	 83% 14% ..
1	G	320	 85% 12% ..
1	H	320	 81% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20717 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 Alpha/beta hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2518	1588	432	492	6			
1	B	316	Total	C	N	O	S	0	0	0
			2527	1594	434	493	6			
1	C	314	Total	C	N	O	S	0	0	0
			2511	1584	432	489	6			
1	D	313	Total	C	N	O	S	0	0	0
			2502	1578	430	488	6			
1	E	316	Total	C	N	O	S	0	0	0
			2526	1593	433	493	7			
1	F	315	Total	C	N	O	S	0	0	0
			2518	1588	432	492	6			
1	G	316	Total	C	N	O	S	0	0	0
			2527	1594	434	493	6			
1	H	314	Total	C	N	O	S	0	0	0
			2511	1583	431	491	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5M9R5N4
A	-1	SER	-	expression tag	UNP A0A5M9R5N4
A	0	HIS	-	expression tag	UNP A0A5M9R5N4
A	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4
B	-2	GLY	-	expression tag	UNP A0A5M9R5N4
B	-1	SER	-	expression tag	UNP A0A5M9R5N4
B	0	HIS	-	expression tag	UNP A0A5M9R5N4
B	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4
C	-2	GLY	-	expression tag	UNP A0A5M9R5N4
C	-1	SER	-	expression tag	UNP A0A5M9R5N4
C	0	HIS	-	expression tag	UNP A0A5M9R5N4
C	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4
D	-2	GLY	-	expression tag	UNP A0A5M9R5N4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP A0A5M9R5N4
D	0	HIS	-	expression tag	UNP A0A5M9R5N4
D	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4
E	-2	GLY	-	expression tag	UNP A0A5M9R5N4
E	-1	SER	-	expression tag	UNP A0A5M9R5N4
E	0	HIS	-	expression tag	UNP A0A5M9R5N4
E	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4
F	-2	GLY	-	expression tag	UNP A0A5M9R5N4
F	-1	SER	-	expression tag	UNP A0A5M9R5N4
F	0	HIS	-	expression tag	UNP A0A5M9R5N4
F	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4
G	-2	GLY	-	expression tag	UNP A0A5M9R5N4
G	-1	SER	-	expression tag	UNP A0A5M9R5N4
G	0	HIS	-	expression tag	UNP A0A5M9R5N4
G	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4
H	-2	GLY	-	expression tag	UNP A0A5M9R5N4
H	-1	SER	-	expression tag	UNP A0A5M9R5N4
H	0	HIS	-	expression tag	UNP A0A5M9R5N4
H	207	ALA	PHE	engineered mutation	UNP A0A5M9R5N4

- Molecule 2 is water.

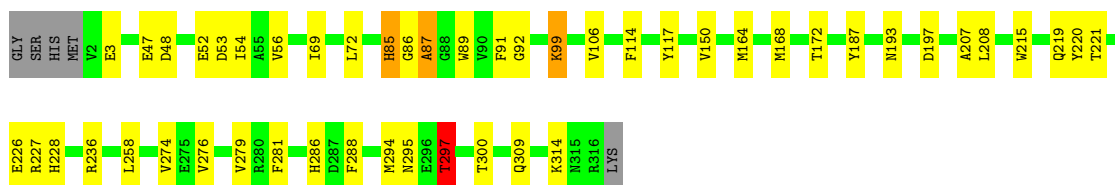
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	97	Total O 97 97	0	0
2	B	76	Total O 76 76	0	0
2	C	39	Total O 39 39	0	0
2	D	43	Total O 43 43	0	0
2	E	72	Total O 72 72	0	0
2	F	73	Total O 73 73	0	0
2	G	107	Total O 107 107	0	0
2	H	70	Total O 70 70	0	0

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.

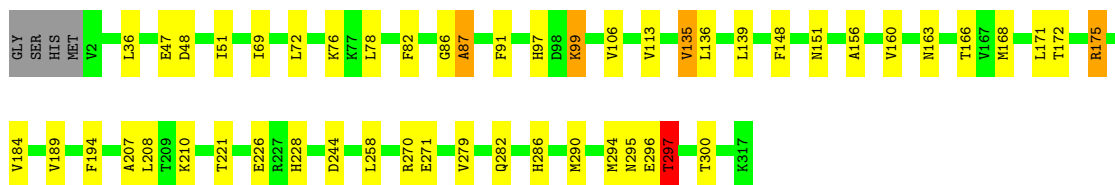
- Molecule 1: Alpha/beta hydrolase

Chain A: 



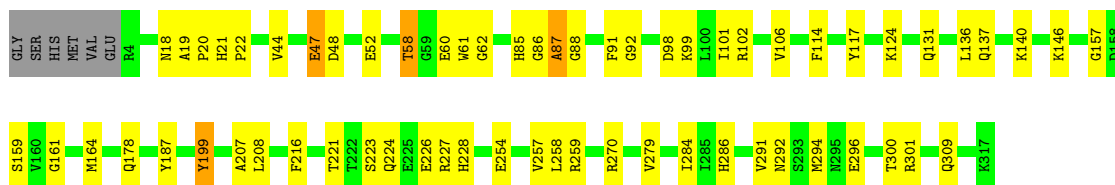
- Molecule 1: Alpha/beta hydrolase

Chain B: 



- Molecule 1: Alpha/beta hydrolase

Chain C: 



- Molecule 1: Alpha/beta hydrolase

Chain D: 





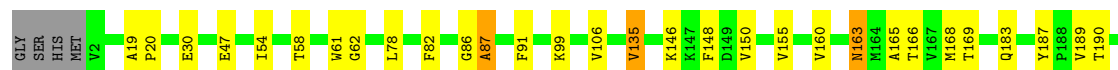
- Molecule 1: Alpha/beta hydrolase

Chain E: 82% 15% ..



- Molecule 1: Alpha/beta hydrolase

Chain F: 83% 14% ..



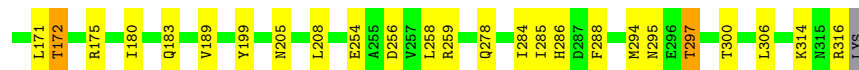
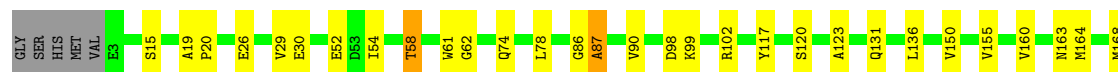
- Molecule 1: Alpha/beta hydrolase

Chain G: 85% 12% ..



- Molecule 1: Alpha/beta hydrolase

Chain H: 81% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.20Å 127.39Å 104.76Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	29.36 – 2.10 29.36 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.36-2.10) 99.9 (29.36-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.245 0.198 , 0.248	Depositor DCC
R_{free} test set	7581 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 21.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20717	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	1.07	0/2570	1.40	6/3491 (0.2%)
1	B	1.06	0/2579	1.44	3/3502 (0.1%)
1	C	1.07	0/2563	1.45	6/3480 (0.2%)
1	D	1.06	0/2554	1.46	5/3469 (0.1%)
1	E	1.03	0/2578	1.41	2/3501 (0.1%)
1	F	1.07	1/2570 (0.0%)	1.43	1/3491 (0.0%)
1	G	1.04	0/2579	1.39	2/3502 (0.1%)
1	H	1.04	1/2563 (0.0%)	1.42	3/3481 (0.1%)
All	All	1.06	2/20556 (0.0%)	1.43	28/27917 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	285	ILE	C-O	6.50	1.30	1.23
1	F	163	ASN	C-O	5.52	1.30	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	ARG	CA-C-O	-7.23	108.50	120.80
1	C	187	TYR	CB-CA-C	7.21	116.32	111.20
1	A	92	GLY	CA-C-O	-7.02	117.38	122.23
1	A	187	TYR	CB-CA-C	6.24	115.63	111.20
1	C	284	ILE	CA-C-N	5.76	128.44	122.27
1	C	284	ILE	C-N-CA	5.76	128.44	122.27
1	H	288	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	297	THR	CB-CA-C	5.45	118.47	109.70
1	B	296	GLU	CA-C-N	5.40	128.51	120.90
1	B	296	GLU	C-N-CA	5.40	128.51	120.90
1	D	161	GLY	CA-C-N	5.33	125.89	119.98
1	D	161	GLY	C-N-CA	5.33	125.89	119.98
1	A	297	THR	CB-CA-C	5.29	119.00	109.64
1	A	85	HIS	CA-C-N	5.24	128.32	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	HIS	C-N-CA	5.24	128.32	122.55
1	A	288	PHE	CA-CB-CG	5.21	119.01	113.80
1	E	202	PHE	CA-C-N	5.20	127.50	120.38
1	E	202	PHE	C-N-CA	5.20	127.50	120.38
1	C	18	ASN	CA-C-N	5.16	126.18	119.78
1	C	18	ASN	C-N-CA	5.16	126.18	119.78
1	F	187	TYR	CB-CA-C	5.09	114.82	111.20
1	H	284	ILE	CA-C-N	5.03	127.66	122.27
1	H	284	ILE	C-N-CA	5.03	127.66	122.27
1	G	202	PHE	CA-C-N	5.02	127.26	120.38
1	G	202	PHE	C-N-CA	5.02	127.26	120.38
1	C	92	GLY	CA-C-O	-5.01	118.77	122.23
1	D	211	GLU	CA-C-N	5.01	125.64	120.03
1	D	211	GLU	C-N-CA	5.01	125.64	120.03

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	2518	0	2444	33	0
1	B	2527	0	2457	33	0
1	C	2511	0	2442	33	0
1	D	2502	0	2429	34	0
1	E	2526	0	2456	36	0
1	F	2518	0	2444	31	0
1	G	2527	0	2457	30	0
1	H	2511	0	2435	32	0
2	A	97	0	0	5	0
2	B	76	0	0	4	0
2	C	39	0	0	2	0
2	D	43	0	0	1	0
2	E	72	0	0	1	0
2	F	73	0	0	1	0
2	G	107	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	70	0	0	3	0
All	All	20717	0	19564	244	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 (244) 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:E:154:THR:HG22	1:E:182:GLN:HE21	1.05	1.10
1:G:154:THR:HG22	1:G:182:GLN:HE21	1.22	1.02
1:D:168:MET:O	1:D:172:THR:HG23	1.62	0.97
1:H:258:LEU:HD12	1:H:286:HIS:CE1	2.03	0.93
1:G:154:THR:HG23	2:G:469:HOH:O	1.70	0.91
1:H:168:MET:O	1:H:172:THR:HG23	1.68	0.91
1:B:297:THR:HG22	1:B:300:THR:H	1.36	0.90
1:A:297:THR:HG22	1:A:300:THR:H	1.37	0.89
1:H:297:THR:HG22	1:H:300:THR:H	1.38	0.88
1:A:168:MET:O	1:A:172:THR:HG23	1.73	0.86
1:E:154:THR:HG22	1:E:182:GLN:NE2	1.90	0.86
1:E:154:THR:HG23	2:E:426:HOH:O	1.78	0.83
1:C:270:ARG:HD3	2:C:426:HOH:O	1.83	0.78
1:H:98:ASP:OD1	1:H:102:ARG:HD2	1.86	0.76
2:A:495:HOH:O	1:G:309:GLN:HG2	1.90	0.71
1:E:279:VAL:CG1	1:F:279:VAL:HG13	2.20	0.71
1:E:279:VAL:HG13	1:F:279:VAL:CG1	2.22	0.69
1:G:154:THR:HG22	1:G:182:GLN:NE2	2.04	0.68
1:B:294:MET:O	1:B:297:THR:HB	1.94	0.68
1:A:221:THR:OG1	1:A:226:GLU:OE1	2.11	0.68
1:F:82:PHE:HE1	1:F:135:VAL:HG22	1.60	0.67
1:C:58:THR:HB	1:C:62:GLY:O	1.93	0.66
1:C:87:ALA:HB1	1:C:91:PHE:HB2	1.78	0.66
1:B:172:THR:CG2	2:B:440:HOH:O	2.44	0.66
1:E:47:GLU:HB3	1:E:106:VAL:HG21	1.78	0.66
1:D:258:LEU:HD12	1:D:286:HIS:CE1	2.32	0.65
1:C:258:LEU:HD12	1:C:286:HIS:CE1	2.32	0.65
1:B:297:THR:HG22	1:B:300:THR:N	2.11	0.64
1:F:287:ASP:HB3	1:F:290:MET:HE2	1.78	0.64
1:D:297:THR:HG22	1:D:300:THR:H	1.63	0.64
1:B:270:ARG:HD3	2:B:417:HOH:O	1.98	0.63
1:A:279:VAL:HG13	1:G:279:VAL:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:VAL:HG13	1:F:279:VAL:HG13	1.79	0.62
1:B:258:LEU:HD12	1:B:286:HIS:CE1	2.33	0.62
1:E:258:LEU:HD12	1:E:286:HIS:CE1	2.35	0.62
1:C:52:GLU:OE1	1:C:146:LYS:NZ	2.33	0.62
1:E:279:VAL:CG1	1:F:279:VAL:CG1	2.78	0.61
1:B:282:GLN:HB2	1:H:278:GLN:HE21	1.65	0.60
1:H:297:THR:HG22	1:H:300:THR:N	2.15	0.59
1:A:227:ARG:O	1:A:236:ARG:NH1	2.36	0.59
1:H:58:THR:HG22	1:H:62:GLY:O	2.02	0.59
1:G:24:ILE:HG12	1:G:91:PHE:CE2	2.38	0.58
1:G:99:LYS:HD2	1:G:295:ASN:OD1	2.03	0.58
1:H:306:LEU:HD12	2:H:460:HOH:O	2.02	0.58
1:F:58:THR:HG21	1:F:61:TRP:HB2	1.86	0.58
1:D:69:ILE:CD1	1:D:101:ILE:HD12	2.34	0.58
1:G:154:THR:CG2	1:G:182:GLN:HE21	2.09	0.57
1:F:258:LEU:HD12	1:F:286:HIS:CE1	2.39	0.57
1:G:52:GLU:CD	1:G:54:ILE:HD11	2.29	0.57
1:C:279:VAL:HG13	1:D:279:VAL:CG2	2.35	0.57
1:A:309:GLN:HG3	1:G:309:GLN:OE1	2.05	0.57
1:H:294:MET:O	1:H:297:THR:HB	2.04	0.57
1:C:85:HIS:HB3	1:C:114:PHE:CE2	2.40	0.56
1:A:279:VAL:HG13	1:G:279:VAL:HG13	1.87	0.56
1:H:74:GLN:HG3	1:H:78:LEU:HD21	1.87	0.56
1:F:228:HIS:ND1	1:F:236:ARG:NH1	2.53	0.56
1:D:270:ARG:HD3	2:D:419:HOH:O	2.04	0.56
1:B:172:THR:HG22	2:B:440:HOH:O	2.03	0.56
1:C:159:SER:HG	1:C:286:HIS:CE1	2.23	0.56
1:E:298:HIS:CE1	1:F:275:GLU:HG2	2.41	0.55
1:B:97:HIS:CE1	1:B:290:MET:HE3	2.41	0.55
1:H:136:LEU:HD21	1:H:180:ILE:HD11	1.89	0.55
1:A:87:ALA:HB1	1:A:91:PHE:HB2	1.89	0.54
1:F:99:LYS:HD2	1:F:295:ASN:OD1	2.06	0.54
1:D:54:ILE:HD12	1:D:68:PHE:CE1	2.42	0.54
1:B:172:THR:HG21	2:B:440:HOH:O	2.05	0.53
1:E:154:THR:CG2	1:E:182:GLN:HE21	1.99	0.53
1:G:3:GLU:O	1:G:3:GLU:HG2	2.09	0.53
1:H:297:THR:CG2	1:H:300:THR:H	2.18	0.53
1:A:52:GLU:OE2	1:A:54:ILE:HD11	2.08	0.53
1:A:294:MET:O	1:A:297:THR:HB	2.08	0.53
1:F:82:PHE:CE1	1:F:135:VAL:HG22	2.42	0.53
1:D:155:VAL:HG11	1:D:180:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:OG1	1:B:226:GLU:OE2	2.22	0.52
1:C:140:LYS:HB2	1:C:178:GLN:HE22	1.73	0.52
1:D:54:ILE:HD12	1:D:68:PHE:CD1	2.45	0.52
1:C:47:GLU:HG3	1:C:106:VAL:HG21	1.91	0.52
1:E:85:HIS:HB3	1:E:114:PHE:CZ	2.44	0.52
1:F:221:THR:HA	2:F:438:HOH:O	2.09	0.52
1:D:47:GLU:HB3	1:D:106:VAL:HG21	1.92	0.52
1:H:120:SER:HA	1:H:123:ALA:O	2.10	0.52
1:A:279:VAL:CG1	1:G:279:VAL:HG13	2.41	0.51
1:C:254:GLU:O	1:C:259:ARG:HD3	2.10	0.51
1:A:236:ARG:NH2	2:A:406:HOH:O	2.43	0.51
1:H:52:GLU:OE2	1:H:54:ILE:HD11	2.10	0.51
1:F:163:ASN:HB2	1:F:189:VAL:O	2.11	0.51
1:H:99:LYS:HD2	1:H:295:ASN:OD1	2.11	0.51
1:G:87:ALA:HB1	1:G:91:PHE:HB2	1.91	0.51
1:A:258:LEU:HD12	1:A:286:HIS:CE1	2.46	0.50
1:D:80:VAL:HG13	1:D:153:LEU:HD13	1.92	0.50
1:C:58:THR:HG21	1:C:131:GLN:HG2	1.93	0.50
1:E:215:TRP:O	1:E:219:GLN:HG2	2.11	0.50
1:E:47:GLU:O	1:E:102:ARG:HD3	2.11	0.50
1:A:52:GLU:CD	1:A:54:ILE:HD11	2.37	0.50
1:D:88:GLY:O	1:D:89:TRP:HB2	2.12	0.50
1:H:171:LEU:O	1:H:175:ARG:HG3	2.12	0.50
1:D:67:ARG:HD2	1:D:94:ALA:HB1	1.94	0.49
1:B:47:GLU:HB3	1:B:106:VAL:HG21	1.94	0.49
1:E:52:GLU:OE1	1:E:146:LYS:HE3	2.12	0.49
1:E:228:HIS:CE1	1:E:236:ARG:NH1	2.81	0.49
1:A:193:ASN:HB2	2:A:406:HOH:O	2.13	0.49
1:B:163:ASN:O	1:B:166:THR:HG22	2.13	0.49
1:E:208:LEU:HD22	1:E:286:HIS:CD2	2.48	0.49
1:B:194:PHE:O	1:B:210:LYS:HE3	2.13	0.48
1:H:314:LYS:HG2	2:H:435:HOH:O	2.12	0.48
1:B:113:VAL:HG11	1:B:139:LEU:HD21	1.96	0.48
1:F:58:THR:O	1:F:58:THR:HG22	2.13	0.48
1:D:249:LEU:HD11	1:D:306:LEU:HD21	1.95	0.48
1:B:171:LEU:O	1:B:175:ARG:HG3	2.14	0.48
1:F:165:ALA:O	1:F:168:MET:HB2	2.14	0.48
1:G:208:LEU:HD22	1:G:286:HIS:CD2	2.49	0.48
1:F:86:GLY:HA2	1:F:160:VAL:HG22	1.96	0.48
1:H:26:GLU:HA	2:H:419:HOH:O	2.13	0.48
1:B:221:THR:HG23	1:B:221:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:HIS:CE1	1:E:236:ARG:HH12	2.32	0.47
1:F:87:ALA:HB1	1:F:91:PHE:HB2	1.95	0.47
1:A:47:GLU:HB3	1:A:106:VAL:HG21	1.96	0.47
1:C:208:LEU:HD22	1:C:286:HIS:CD2	2.50	0.47
1:F:86:GLY:HA2	1:F:160:VAL:CG2	2.44	0.47
1:C:301:ARG:HA	1:C:301:ARG:NE	2.29	0.47
1:A:279:VAL:CG1	1:G:279:VAL:CG1	2.93	0.47
1:D:69:ILE:O	1:D:111:VAL:HA	2.15	0.47
1:B:86:GLY:HA2	1:B:160:VAL:HG22	1.97	0.47
1:D:164:MET:O	1:D:168:MET:HG2	2.14	0.47
1:E:156:ALA:HA	1:E:184:VAL:O	2.15	0.47
1:F:287:ASP:HB3	1:F:290:MET:CE	2.44	0.47
1:G:81:ILE:HG12	1:G:154:THR:OG1	2.14	0.47
1:G:133:TYR:O	1:G:137:GLN:HG2	2.15	0.47
1:F:58:THR:HB	1:F:62:GLY:O	2.15	0.47
1:H:163:ASN:HB2	1:H:189:VAL:O	2.15	0.47
1:C:300:THR:HG22	1:C:301:ARG:NH1	2.30	0.46
1:E:199:TYR:CD1	1:E:257:VAL:HB	2.50	0.46
1:G:171:LEU:O	1:G:175:ARG:HG3	2.15	0.46
1:B:48:ASP:HB3	1:B:72:LEU:HD11	1.96	0.46
1:B:208:LEU:HD22	1:B:286:HIS:CD2	2.49	0.46
1:E:298:HIS:CE1	1:F:275:GLU:CG	2.99	0.46
1:D:191:ASP:HB2	1:D:235:LEU:HD23	1.98	0.46
1:C:224:GLN:HG3	1:C:228:HIS:CE1	2.51	0.46
1:G:267:ARG:O	1:G:271:GLU:HG2	2.16	0.46
1:D:93:ASN:OD1	1:D:95:HIS:HB3	2.16	0.45
1:C:98:ASP:CG	1:C:102:ARG:HE	2.24	0.45
1:E:58:THR:HB	1:E:62:GLY:O	2.17	0.45
1:A:314:LYS:HG2	2:A:451:HOH:O	2.15	0.45
1:C:58:THR:CG2	1:C:61:TRP:HB2	2.47	0.45
1:E:224:GLN:OE1	1:E:224:GLN:HA	2.17	0.45
1:A:86:GLY:O	1:A:87:ALA:HB3	2.17	0.45
1:B:156:ALA:HA	1:B:184:VAL:O	2.17	0.45
1:E:129:ILE:O	1:E:168:MET:HE1	2.17	0.45
1:H:15:SER:HB3	1:H:205:ASN:O	2.16	0.45
1:H:254:GLU:O	1:H:259:ARG:HD3	2.16	0.45
1:E:19:ALA:HB3	1:E:20:PRO:HD3	1.99	0.45
1:H:19:ALA:N	1:H:20:PRO:CD	2.80	0.45
1:A:85:HIS:HB3	1:A:114:PHE:CZ	2.52	0.44
1:B:51:ILE:HG12	1:B:69:ILE:HG22	1.98	0.44
1:C:19:ALA:N	1:C:20:PRO:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:HD2	1:B:295:ASN:OD1	2.17	0.44
1:E:58:THR:HG21	1:E:61:TRP:HB2	1.99	0.44
1:H:208:LEU:HD22	1:H:286:HIS:CD2	2.52	0.44
1:D:155:VAL:CG1	1:D:180:ILE:HD13	2.47	0.44
1:C:86:GLY:O	1:C:87:ALA:HB3	2.17	0.44
1:D:11:ALA:HB2	1:D:284:ILE:HD12	1.99	0.44
1:D:56:VAL:HG11	1:D:135:VAL:HG22	2.00	0.44
1:G:163:ASN:HB2	1:G:189:VAL:O	2.17	0.44
1:H:86:GLY:O	1:H:87:ALA:HB3	2.17	0.44
1:D:284:ILE:CD1	1:D:297:THR:HG21	2.47	0.44
1:A:53:ASP:O	2:A:401:HOH:O	2.21	0.44
1:A:309:GLN:HG3	1:G:309:GLN:CD	2.43	0.44
1:B:82:PHE:CD2	1:B:136:LEU:HD13	2.52	0.44
1:B:86:GLY:O	1:B:87:ALA:HB3	2.18	0.44
1:H:117:TYR:CZ	1:H:164:MET:HE1	2.53	0.44
1:H:160:VAL:O	1:H:163:ASN:HB3	2.18	0.44
1:A:99:LYS:HD2	1:A:295:ASN:OD1	2.18	0.43
1:H:58:THR:CG2	1:H:61:TRP:HB2	2.47	0.43
1:A:215:TRP:O	1:A:219:GLN:HG2	2.18	0.43
1:A:297:THR:CG2	1:A:300:THR:H	2.19	0.43
1:C:279:VAL:HG13	1:D:279:VAL:HG23	1.99	0.43
1:D:85:HIS:HB3	1:D:114:PHE:CZ	2.53	0.43
1:D:117:TYR:CZ	1:D:164:MET:HE1	2.53	0.43
1:C:136:LEU:HB3	1:C:137:GLN:NE2	2.34	0.43
1:E:169:THR:HB	1:E:246:PRO:HD2	1.99	0.43
1:F:190:THR:OG1	1:F:261:GLU:HG3	2.18	0.43
1:F:47:GLU:HB3	1:F:106:VAL:HG21	2.01	0.43
1:H:256:ASP:CG	1:H:286:HIS:HD1	2.25	0.43
1:B:244:ASP:OD2	1:D:9:LYS:NZ	2.50	0.43
1:C:88:GLY:HA3	1:C:216:PHE:CD1	2.54	0.43
1:G:82:PHE:CE1	1:G:135:VAL:HG22	2.54	0.43
1:A:274:VAL:O	1:A:276:VAL:HG23	2.19	0.43
1:C:221:THR:OG1	1:C:226:GLU:OE1	2.26	0.43
1:D:90:VAL:HA	1:D:120:SER:O	2.19	0.43
1:E:54:ILE:HD12	1:E:68:PHE:CD1	2.53	0.43
1:E:171:LEU:O	1:E:175:ARG:HG3	2.18	0.43
1:H:58:THR:CG2	1:H:62:GLY:O	2.67	0.43
1:B:36:LEU:HD21	1:B:290:MET:HE1	2.00	0.43
1:B:82:PHE:CE1	1:B:135:VAL:HG22	2.54	0.43
1:E:69:ILE:CD1	1:E:101:ILE:HD12	2.49	0.43
1:F:58:THR:CG2	1:F:61:TRP:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:VAL:HG13	1:H:90:VAL:CG1	2.48	0.43
1:E:163:ASN:O	1:E:167:VAL:HG23	2.18	0.42
1:G:88:GLY:O	1:G:89:TRP:HB2	2.18	0.42
1:G:215:TRP:O	1:G:219:GLN:HG2	2.19	0.42
1:C:21:HIS:HA	1:C:22:PRO:C	2.44	0.42
1:C:223:SER:O	1:C:227:ARG:HG3	2.18	0.42
1:C:44:VAL:HB	1:C:292:ASN:HB3	2.01	0.42
1:E:310:TRP:CZ2	1:E:314:LYS:HE3	2.54	0.42
1:C:117:TYR:CZ	1:C:164:MET:HE1	2.55	0.42
1:A:117:TYR:CZ	1:A:164:MET:HE1	2.54	0.42
1:C:19:ALA:N	1:C:20:PRO:CD	2.83	0.42
1:E:82:PHE:CE1	1:E:135:VAL:HG22	2.54	0.42
1:E:185:LEU:HD12	1:E:250:ILE:HG12	2.01	0.42
1:B:78:LEU:O	1:B:148:PHE:HA	2.20	0.42
1:G:254:GLU:O	1:G:259:ARG:HD3	2.20	0.42
1:B:163:ASN:HB2	1:B:189:VAL:O	2.20	0.42
1:F:155:VAL:O	1:F:183:GLN:HA	2.20	0.41
1:B:151:ASN:HB3	1:D:43:PRO:HD3	2.02	0.41
1:B:168:MET:O	1:B:172:THR:HG23	2.20	0.41
1:F:58:THR:O	1:F:58:THR:CG2	2.68	0.41
1:A:89:TRP:CD1	1:A:220:TYR:CE1	3.08	0.41
1:D:199:TYR:O	1:D:203:ALA:HB2	2.20	0.41
1:E:44:VAL:HG21	1:E:99:LYS:HD3	2.02	0.41
1:A:48:ASP:HB3	1:A:72:LEU:HD11	2.02	0.41
1:D:86:GLY:O	1:D:87:ALA:HB3	2.21	0.41
1:E:195:ASP:OD1	1:E:195:ASP:N	2.52	0.41
1:F:19:ALA:N	1:F:20:PRO:CD	2.83	0.41
1:D:159:SER:HA	1:D:187:TYR:O	2.20	0.41
1:D:202:PHE:HD1	1:D:206:TYR:CE2	2.39	0.41
1:A:85:HIS:HB3	1:A:114:PHE:CE2	2.55	0.41
1:A:208:LEU:HD22	1:A:286:HIS:CD2	2.55	0.41
1:C:199:TYR:CD1	1:C:257:VAL:HB	2.56	0.41
1:F:274:VAL:O	1:F:276:VAL:HG23	2.20	0.41
1:G:85:HIS:HB3	1:G:114:PHE:CE2	2.55	0.41
1:H:155:VAL:O	1:H:183:GLN:HA	2.20	0.41
1:H:58:THR:HG21	1:H:131:GLN:HG2	2.02	0.41
1:A:228:HIS:CD2	1:A:236:ARG:CZ	3.04	0.40
1:C:157:GLY:HA3	1:C:161:GLY:C	2.46	0.40
1:C:291:VAL:HB	1:C:294:MET:HE3	2.03	0.40
1:G:47:GLU:HB3	1:G:106:VAL:HG21	2.03	0.40
1:A:281:PHE:CD2	1:G:279:VAL:HG22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:TRP:CZ2	1:D:220:TYR:CE2	3.08	0.40
1:C:101:ILE:HD11	2:C:420:HOH:O	2.21	0.40
1:D:191:ASP:HA	1:D:233:SER:HB3	2.03	0.40
1:F:78:LEU:O	1:F:148:PHE:HA	2.21	0.40
1:G:223:SER:C	1:G:224:GLN:HG2	2.46	0.40
1:B:87:ALA:HB1	1:B:91:PHE:HB2	2.04	0.40
1:F:169:THR:HB	1:F:246:PRO:HD2	2.02	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	313/320 (98%)	299 (96%)	12 (4%)	2 (1%)	21	18
1	B	314/320 (98%)	294 (94%)	18 (6%)	2 (1%)	21	18
1	C	312/320 (98%)	294 (94%)	16 (5%)	2 (1%)	21	18
1	D	311/320 (97%)	290 (93%)	19 (6%)	2 (1%)	21	18
1	E	314/320 (98%)	303 (96%)	10 (3%)	1 (0%)	36	36
1	F	313/320 (98%)	298 (95%)	12 (4%)	3 (1%)	12	9
1	G	314/320 (98%)	299 (95%)	13 (4%)	2 (1%)	21	18
1	H	312/320 (98%)	297 (95%)	14 (4%)	1 (0%)	36	36
All	All	2503/2560 (98%)	2374 (95%)	114 (5%)	15 (1%)	21	18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	ALA
1	C	207	ALA
1	A	87	ALA

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Mol	Chain	Res	Type
1	D	87	ALA
1	D	207	ALA
1	F	87	ALA
1	H	87	ALA
1	C	87	ALA
1	E	87	ALA
1	F	205	ASN
1	G	87	ALA
1	B	207	ALA
1	G	207	ALA
1	F	207	ALA
1	A	207	ALA

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	270/274 (98%)	263 (97%)	7 (3%)	40	46
1	B	271/274 (99%)	263 (97%)	8 (3%)	36	41
1	C	269/274 (98%)	260 (97%)	9 (3%)	33	37
1	D	268/274 (98%)	264 (98%)	4 (2%)	57	65
1	E	271/274 (99%)	265 (98%)	6 (2%)	45	53
1	F	270/274 (98%)	261 (97%)	9 (3%)	33	37
1	G	271/274 (99%)	262 (97%)	9 (3%)	33	37
1	H	269/274 (98%)	262 (97%)	7 (3%)	40	46
All	All	2159/2192 (98%)	2100 (97%)	59 (3%)	39	45

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	56	VAL
1	A	69	ILE

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Mol	Chain	Res	Type
1	A	99	LYS
1	A	150	VAL
1	A	197	ASP
1	A	297	THR
1	B	76	LYS
1	B	99	LYS
1	B	135	VAL
1	B	175	ARG
1	B	228	HIS
1	B	271	GLU
1	B	279	VAL
1	B	297	THR
1	C	47	GLU
1	C	48	ASP
1	C	58	THR
1	C	60	GLU
1	C	99	LYS
1	C	124	LYS
1	C	199	TYR
1	C	296	GLU
1	C	309	GLN
1	D	99	LYS
1	D	199	TYR
1	D	279	VAL
1	D	306	LEU
1	E	1	MET
1	E	56	VAL
1	E	99	LYS
1	E	135	VAL
1	E	154	THR
1	E	199	TYR
1	F	30	GLU
1	F	54	ILE
1	F	135	VAL
1	F	146	LYS
1	F	150	VAL
1	F	166	THR
1	F	199	TYR
1	F	225	GLU
1	F	296	GLU
1	G	24	ILE
1	G	99	LYS

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Mol	Chain	Res	Type
1	G	126	PRO
1	G	135	VAL
1	G	150	VAL
1	G	175	ARG
1	G	199	TYR
1	G	296	GLU
1	G	317	LYS
1	H	30	GLU
1	H	58	THR
1	H	150	VAL
1	H	172	THR
1	H	199	TYR
1	H	297	THR
1	H	316	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	182	GLN
1	A	193	ASN
1	A	228	HIS
1	A	298	HIS
1	B	309	GLN
1	C	178	GLN
1	D	178	GLN
1	D	224	GLN
1	D	309	GLN
1	E	182	GLN
1	E	193	ASN
1	E	228	HIS
1	E	298	HIS
1	F	152	HIS
1	F	183	GLN
1	F	224	GLN
1	G	152	HIS
1	G	182	GLN
1	H	193	ASN
1	H	278	GLN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	315/320 (98%)	-1.54	0 100 100	22, 32, 46, 66	0
1	B	316/320 (98%)	-1.51	0 100 100	27, 37, 54, 75	0
1	C	314/320 (98%)	-1.39	0 100 100	33, 46, 62, 82	0
1	D	313/320 (97%)	-1.37	0 100 100	32, 46, 67, 82	0
1	E	316/320 (98%)	-1.56	0 100 100	24, 33, 50, 80	0
1	F	315/320 (98%)	-1.54	0 100 100	25, 33, 51, 64	0
1	G	316/320 (98%)	-1.56	0 100 100	22, 33, 51, 72	0
1	H	314/320 (98%)	-1.48	0 100 100	25, 37, 55, 69	0
All	All	2519/2560 (98%)	-1.49	0 100 100	22, 37, 57, 82	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.