



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:58 AM UTC

PDB ID : 5EGN / pdb_00005egn
Title : Est816 as an N-Acyl homoserine lactone degrading enzyme
Authors : Xie, W.; Liu, X.; Cao, L.; Liu, Y.
Deposited on : 2015-10-27
Resolution : 2.64 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

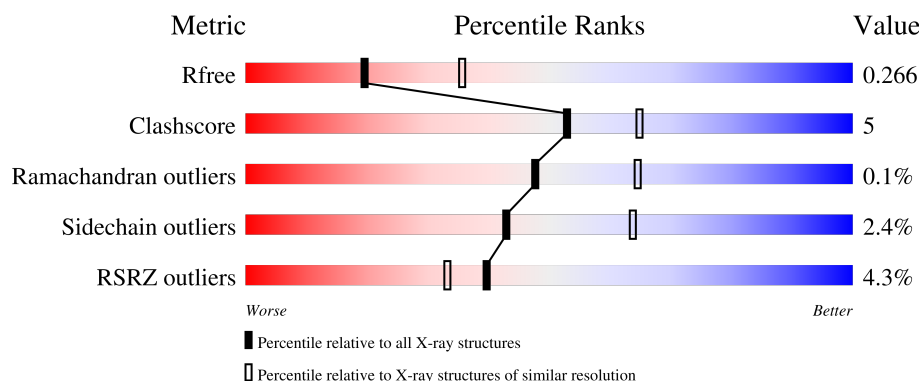
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	271	
1	B	271	
1	C	271	
1	D	271	
1	E	271	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	271	2% 83% 13%
1	G	271	11% 82% 13%
1	H	271	10% 79% 14% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16184 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 Esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1983	1264	344	370	5			
1	B	260	Total	C	N	O	S	0	0	0
			1991	1268	345	373	5			
1	C	259	Total	C	N	O	S	0	0	0
			1986	1265	344	372	5			
1	D	259	Total	C	N	O	S	0	0	0
			1980	1259	344	372	5			
1	E	259	Total	C	N	O	S	0	0	0
			1980	1259	344	372	5			
1	F	260	Total	C	N	O	S	0	0	0
			1979	1258	345	371	5			
1	G	259	Total	C	N	O	S	0	0	0
			1950	1242	334	369	5			
1	H	258	Total	C	N	O	S	0	0	0
			1935	1233	335	362	5			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	VAL	ALA	engineered mutation	UNP I6YRG4
A	238	ASN	LYS	engineered mutation	UNP I6YRG4
A	262	ALA	-	expression tag	UNP I6YRG4
A	263	ALA	-	expression tag	UNP I6YRG4
A	264	LEU	-	expression tag	UNP I6YRG4
A	265	GLU	-	expression tag	UNP I6YRG4
A	266	HIS	-	expression tag	UNP I6YRG4
A	267	HIS	-	expression tag	UNP I6YRG4
A	268	HIS	-	expression tag	UNP I6YRG4
A	269	HIS	-	expression tag	UNP I6YRG4
A	270	HIS	-	expression tag	UNP I6YRG4
A	271	HIS	-	expression tag	UNP I6YRG4
B	216	VAL	ALA	engineered mutation	UNP I6YRG4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	238	ASN	LYS	engineered mutation	UNP I6YRG4
B	262	ALA	-	expression tag	UNP I6YRG4
B	263	ALA	-	expression tag	UNP I6YRG4
B	264	LEU	-	expression tag	UNP I6YRG4
B	265	GLU	-	expression tag	UNP I6YRG4
B	266	HIS	-	expression tag	UNP I6YRG4
B	267	HIS	-	expression tag	UNP I6YRG4
B	268	HIS	-	expression tag	UNP I6YRG4
B	269	HIS	-	expression tag	UNP I6YRG4
B	270	HIS	-	expression tag	UNP I6YRG4
B	271	HIS	-	expression tag	UNP I6YRG4
C	216	VAL	ALA	engineered mutation	UNP I6YRG4
C	238	ASN	LYS	engineered mutation	UNP I6YRG4
C	262	ALA	-	expression tag	UNP I6YRG4
C	263	ALA	-	expression tag	UNP I6YRG4
C	264	LEU	-	expression tag	UNP I6YRG4
C	265	GLU	-	expression tag	UNP I6YRG4
C	266	HIS	-	expression tag	UNP I6YRG4
C	267	HIS	-	expression tag	UNP I6YRG4
C	268	HIS	-	expression tag	UNP I6YRG4
C	269	HIS	-	expression tag	UNP I6YRG4
C	270	HIS	-	expression tag	UNP I6YRG4
C	271	HIS	-	expression tag	UNP I6YRG4
D	216	VAL	ALA	engineered mutation	UNP I6YRG4
D	238	ASN	LYS	engineered mutation	UNP I6YRG4
D	262	ALA	-	expression tag	UNP I6YRG4
D	263	ALA	-	expression tag	UNP I6YRG4
D	264	LEU	-	expression tag	UNP I6YRG4
D	265	GLU	-	expression tag	UNP I6YRG4
D	266	HIS	-	expression tag	UNP I6YRG4
D	267	HIS	-	expression tag	UNP I6YRG4
D	268	HIS	-	expression tag	UNP I6YRG4
D	269	HIS	-	expression tag	UNP I6YRG4
D	270	HIS	-	expression tag	UNP I6YRG4
D	271	HIS	-	expression tag	UNP I6YRG4
E	216	VAL	ALA	engineered mutation	UNP I6YRG4
E	238	ASN	LYS	engineered mutation	UNP I6YRG4
E	262	ALA	-	expression tag	UNP I6YRG4
E	263	ALA	-	expression tag	UNP I6YRG4
E	264	LEU	-	expression tag	UNP I6YRG4
E	265	GLU	-	expression tag	UNP I6YRG4
E	266	HIS	-	expression tag	UNP I6YRG4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	267	HIS	-	expression tag	UNP I6YRG4
E	268	HIS	-	expression tag	UNP I6YRG4
E	269	HIS	-	expression tag	UNP I6YRG4
E	270	HIS	-	expression tag	UNP I6YRG4
E	271	HIS	-	expression tag	UNP I6YRG4
F	216	VAL	ALA	engineered mutation	UNP I6YRG4
F	238	ASN	LYS	engineered mutation	UNP I6YRG4
F	262	ALA	-	expression tag	UNP I6YRG4
F	263	ALA	-	expression tag	UNP I6YRG4
F	264	LEU	-	expression tag	UNP I6YRG4
F	265	GLU	-	expression tag	UNP I6YRG4
F	266	HIS	-	expression tag	UNP I6YRG4
F	267	HIS	-	expression tag	UNP I6YRG4
F	268	HIS	-	expression tag	UNP I6YRG4
F	269	HIS	-	expression tag	UNP I6YRG4
F	270	HIS	-	expression tag	UNP I6YRG4
F	271	HIS	-	expression tag	UNP I6YRG4
G	216	VAL	ALA	engineered mutation	UNP I6YRG4
G	238	ASN	LYS	engineered mutation	UNP I6YRG4
G	262	ALA	-	expression tag	UNP I6YRG4
G	263	ALA	-	expression tag	UNP I6YRG4
G	264	LEU	-	expression tag	UNP I6YRG4
G	265	GLU	-	expression tag	UNP I6YRG4
G	266	HIS	-	expression tag	UNP I6YRG4
G	267	HIS	-	expression tag	UNP I6YRG4
G	268	HIS	-	expression tag	UNP I6YRG4
G	269	HIS	-	expression tag	UNP I6YRG4
G	270	HIS	-	expression tag	UNP I6YRG4
G	271	HIS	-	expression tag	UNP I6YRG4
H	216	VAL	ALA	engineered mutation	UNP I6YRG4
H	238	ASN	LYS	engineered mutation	UNP I6YRG4
H	262	ALA	-	expression tag	UNP I6YRG4
H	263	ALA	-	expression tag	UNP I6YRG4
H	264	LEU	-	expression tag	UNP I6YRG4
H	265	GLU	-	expression tag	UNP I6YRG4
H	266	HIS	-	expression tag	UNP I6YRG4
H	267	HIS	-	expression tag	UNP I6YRG4
H	268	HIS	-	expression tag	UNP I6YRG4
H	269	HIS	-	expression tag	UNP I6YRG4
H	270	HIS	-	expression tag	UNP I6YRG4
H	271	HIS	-	expression tag	UNP I6YRG4

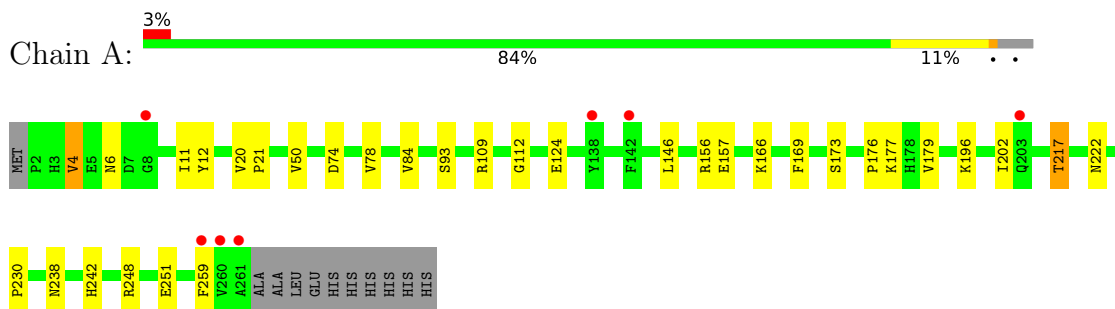
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total 41	O 41	0	0
2	B	67	Total 67	O 67	0	0
2	C	59	Total 59	O 59	0	0
2	D	49	Total 49	O 49	0	0
2	E	58	Total 58	O 58	0	0
2	F	61	Total 61	O 61	0	0
2	G	28	Total 28	O 28	0	0
2	H	37	Total 37	O 37	0	0

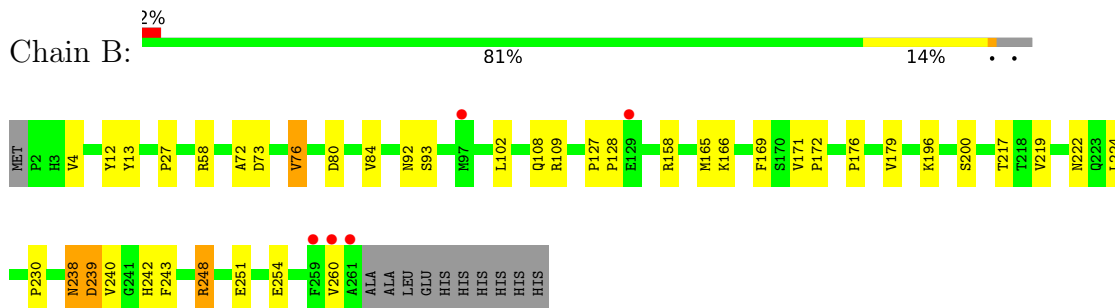
3 Residue-property plots [i](#)

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.

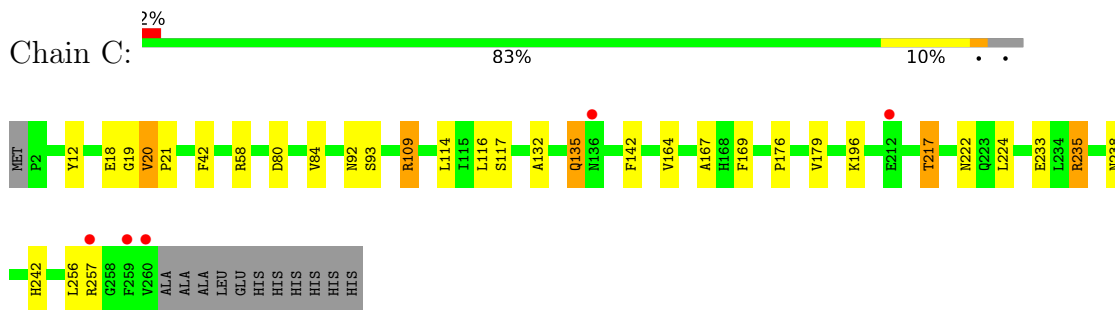
- Molecule 1: Esterase



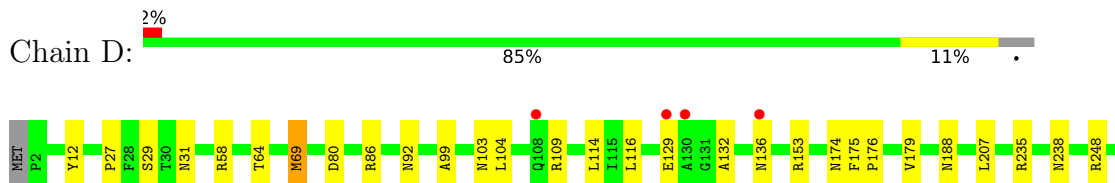
- Molecule 1: Esterase

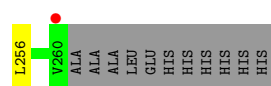


- Molecule 1: Esterase

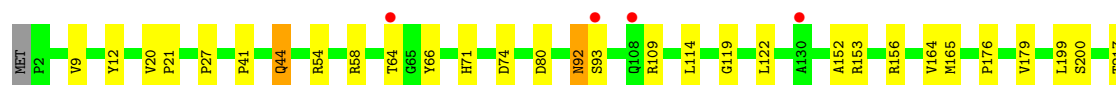
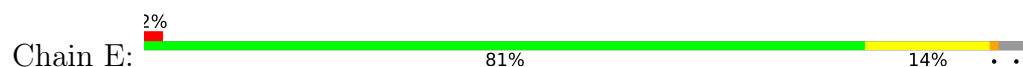


- Molecule 1: Esterase

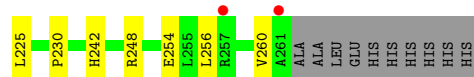
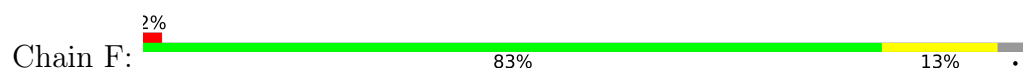




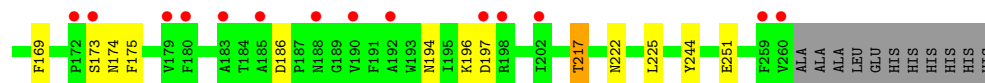
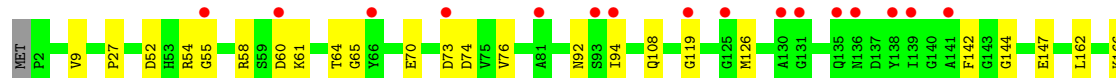
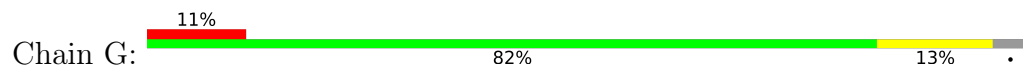
• Molecule 1: Esterase



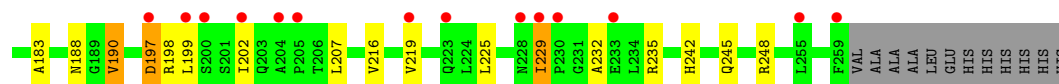
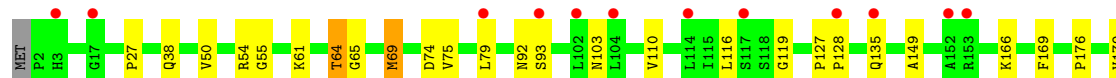
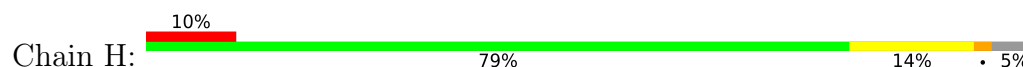
• Molecule 1: Esterase



• Molecule 1: Esterase



• Molecule 1: Esterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.81Å 78.55Å 116.47Å 90.00° 99.37° 90.00°	Depositor
Resolution (Å)	44.82 – 2.64 44.82 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.82-2.64) 91.1 (44.82-2.64)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.219 , 0.264 0.223 , 0.266	Depositor DCC
R_{free} test set	2981 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16184	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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	0.30	0/2033	0.76	2/2767 (0.1%)
1	B	0.31	0/2041	0.78	2/2777 (0.1%)
1	C	0.30	0/2036	0.78	0/2770
1	D	0.30	0/2029	0.78	0/2761
1	E	0.30	0/2029	0.78	0/2761
1	F	0.31	0/2027	0.79	2/2758 (0.1%)
1	G	0.31	0/1997	0.84	4/2720 (0.1%)
1	H	0.34	0/1983	0.82	4/2703 (0.1%)
All	All	0.31	0/16175	0.79	14/22017 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	186	ASP	CA-C-N	7.30	127.46	119.87
1	G	186	ASP	C-N-CA	7.30	127.46	119.87
1	G	126	MET	CA-C-N	-6.52	113.67	120.38
1	G	126	MET	C-N-CA	-6.52	113.67	120.38
1	H	248	ARG	CA-C-N	5.71	125.18	119.24
1	H	248	ARG	C-N-CA	5.71	125.18	119.24
1	H	229	ILE	CA-C-N	5.60	126.84	119.84
1	H	229	ILE	C-N-CA	5.60	126.84	119.84
1	B	248	ARG	CA-C-N	5.34	124.52	118.97
1	B	248	ARG	C-N-CA	5.34	124.52	118.97
1	F	248	ARG	CA-C-N	5.08	124.25	118.97
1	F	248	ARG	C-N-CA	5.08	124.25	118.97
1	A	248	ARG	CA-C-N	5.05	124.49	119.24
1	A	248	ARG	C-N-CA	5.05	124.49	119.24

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	1983	0	1921	16	0
1	B	1991	0	1931	25	0
1	C	1986	0	1926	19	0
1	D	1980	0	1919	18	1
1	E	1980	0	1919	27	0
1	F	1979	0	1914	16	0
1	G	1950	0	1860	21	0
1	H	1935	0	1849	22	0
2	A	41	0	0	1	0
2	B	67	0	0	2	0
2	C	59	0	0	0	0
2	D	49	0	0	1	0
2	E	58	0	0	0	0
2	F	61	0	0	0	0
2	G	28	0	0	3	0
2	H	37	0	0	0	0
All	All	16184	0	15239	156	1

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 5.

All (156) 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:G:55:GLY:O	2:G:301:HOH:O	1.91	0.86
1:E:80:ASP:OD1	1:E:109:ARG:NH2	2.14	0.81
1:G:61:LYS:NZ	1:G:173:SER:O	2.15	0.80
1:H:135:GLN:N	1:H:135:GLN:OE1	2.17	0.76
1:G:174:ASN:O	2:G:301:HOH:O	2.04	0.74
1:D:80:ASP:OD1	1:D:109:ARG:NH2	2.20	0.74
1:F:80:ASP:OD1	1:F:109:ARG:NH2	2.19	0.73
1:D:153:ARG:NH1	1:D:248:ARG:HE	1.89	0.71
1:B:80:ASP:OD1	1:B:109:ARG:NH2	2.24	0.71
1:C:84:VAL:O	1:C:109:ARG:NH1	2.21	0.70
1:C:80:ASP:OD1	1:C:109:ARG:NH2	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:O	1:A:109:ARG:NH2	2.28	0.66
1:D:256:LEU:O	2:D:301:HOH:O	2.14	0.65
1:F:135:GLN:NE2	1:F:181:ASP:OD1	2.29	0.64
1:E:199:LEU:HD23	1:E:228:ASN:HB2	1.80	0.63
1:A:124:GLU:OE2	1:A:196:LYS:NZ	2.32	0.62
1:D:132:ALA:O	1:D:136:ASN:ND2	2.27	0.62
1:G:169:PHE:HA	1:G:175:PHE:HB3	1.81	0.62
1:A:4:VAL:HG21	1:A:78:VAL:HA	1.82	0.61
1:A:251:GLU:OE1	2:A:301:HOH:O	2.17	0.60
1:H:207:LEU:HD11	1:H:235:ARG:HG2	1.85	0.57
1:E:153:ARG:CZ	1:E:248:ARG:HE	2.17	0.57
1:B:84:VAL:O	1:B:109:ARG:NH1	2.37	0.57
1:G:54:ARG:HE	1:G:74:ASP:CG	2.12	0.56
1:E:153:ARG:CZ	1:E:239:ASP:HB3	2.36	0.56
1:B:217:THR:HG22	1:B:222:ASN:HD21	1.71	0.55
1:D:69:MET:HE2	1:D:188:ASN:HB3	1.89	0.54
1:D:31:ASN:ND2	1:D:174:ASN:OD1	2.38	0.54
1:B:176:PRO:HG2	1:B:179:VAL:HG23	1.90	0.53
1:F:200:SER:HA	1:F:230:PRO:HD3	1.91	0.53
1:G:54:ARG:NH1	1:G:70:GLU:OE1	2.41	0.53
1:H:69:MET:N	1:H:69:MET:SD	2.83	0.52
1:G:54:ARG:NH2	1:G:74:ASP:OD1	2.34	0.52
1:G:27:PRO:HD3	1:G:92:ASN:HB3	1.91	0.52
1:A:176:PRO:HG2	1:A:179:VAL:HG23	1.92	0.51
1:B:93:SER:HB2	1:B:242:HIS:NE2	2.25	0.51
1:H:69:MET:HE2	1:H:188:ASN:HB3	1.91	0.51
1:C:233:GLU:OE1	1:C:235:ARG:NH2	2.44	0.51
1:E:41:PRO:O	1:E:44:GLN:HB2	2.11	0.51
1:D:207:LEU:HD11	1:D:235:ARG:HG2	1.92	0.51
1:E:176:PRO:HG2	1:E:179:VAL:HG23	1.93	0.51
1:H:119:GLY:HA2	1:H:225:LEU:HD11	1.93	0.51
1:G:175:PHE:HA	2:G:301:HOH:O	2.10	0.51
1:B:158:ARG:NH1	2:B:303:HOH:O	2.31	0.50
1:C:176:PRO:HG2	1:C:179:VAL:HG23	1.94	0.50
1:E:122:LEU:HD21	1:E:217:THR:HG22	1.94	0.50
1:G:119:GLY:HA2	1:G:225:LEU:HD11	1.93	0.50
1:G:73:ASP:HA	1:G:76:VAL:HG12	1.93	0.50
1:A:217:THR:HG22	1:A:222:ASN:HD21	1.78	0.49
1:B:76:VAL:HG12	1:B:102:LEU:HD11	1.95	0.49
1:B:166:LYS:HA	1:B:169:PHE:CE2	2.48	0.49
1:B:4:VAL:HG13	1:B:13:TYR:HE1	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:ARG:HG2	1:F:71:HIS:CE1	2.47	0.48
1:G:54:ARG:NE	1:G:74:ASP:OD2	2.39	0.48
1:F:183:ALA:HB1	1:F:190:VAL:HG23	1.94	0.48
1:D:27:PRO:HB3	1:D:92:ASN:OD1	2.14	0.48
1:E:153:ARG:NH2	1:E:248:ARG:HE	2.11	0.48
1:C:217:THR:HG22	1:C:222:ASN:HD21	1.79	0.47
1:E:54:ARG:HD2	1:E:74:ASP:OD2	2.13	0.47
1:H:103:ASN:HD21	1:H:110:VAL:HG11	1.79	0.47
1:F:93:SER:HB2	1:F:242:HIS:NE2	2.29	0.47
1:E:248:ARG:NH1	1:E:251:GLU:OE1	2.47	0.47
1:F:176:PRO:HG2	1:F:179:VAL:HG23	1.97	0.47
1:C:12:TYR:OH	1:E:58:ARG:HD3	2.14	0.47
1:F:123:GLY:HA2	1:F:126:MET:HE2	1.96	0.47
1:H:229:ILE:HB	1:H:232:ALA:HB2	1.96	0.46
1:F:114:LEU:HD13	1:F:256:LEU:HD13	1.98	0.46
1:F:119:GLY:HA2	1:F:225:LEU:HD11	1.97	0.46
1:H:166:LYS:HA	1:H:169:PHE:CE2	2.51	0.46
1:A:173:SER:HB2	1:F:16:TYR:HD1	1.81	0.46
1:E:27:PRO:HB3	1:E:92:ASN:HD22	1.81	0.46
1:C:42:PHE:CE1	1:C:257:ARG:HG3	2.50	0.46
1:D:153:ARG:HH12	1:D:248:ARG:HE	1.63	0.46
1:B:196:LYS:HG2	1:B:224:LEU:HD21	1.98	0.45
1:D:176:PRO:HG2	1:D:179:VAL:HG23	1.98	0.45
1:A:166:LYS:HA	1:A:169:PHE:CE2	2.51	0.45
1:E:54:ARG:HG2	1:E:71:HIS:CE1	2.51	0.45
1:F:54:ARG:HD2	1:F:74:ASP:OD2	2.16	0.45
1:H:176:PRO:HG2	1:H:179:VAL:HG23	1.99	0.45
1:E:164:VAL:HG13	1:E:165:MET:HE2	1.99	0.45
1:G:9:VAL:HG13	1:G:60:ASP:HB2	1.98	0.45
1:A:12:TYR:OH	1:F:58:ARG:HD3	2.16	0.45
1:C:92:ASN:ND2	1:C:116:LEU:O	2.42	0.45
1:D:92:ASN:HD22	1:D:116:LEU:HD23	1.82	0.45
1:B:165:MET:HE3	1:B:243:PHE:CG	2.52	0.45
1:C:93:SER:HB2	1:C:242:HIS:NE2	2.32	0.44
1:D:114:LEU:HD13	1:D:256:LEU:HD13	2.00	0.44
1:E:200:SER:HA	1:E:230:PRO:HD3	1.99	0.44
1:A:202:ILE:O	1:A:230:PRO:HD2	2.17	0.44
1:B:73:ASP:HA	1:B:76:VAL:HG13	1.99	0.44
1:H:149:ALA:HB2	1:H:216:VAL:HG21	2.00	0.44
1:B:248:ARG:HE	1:B:251:GLU:CD	2.26	0.44
1:B:58:ARG:NH2	2:B:309:HOH:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:ALA:HB1	1:H:190:VAL:HG23	1.99	0.44
1:B:238:ASN:HA	1:B:239:ASP:HA	1.77	0.43
1:A:156:ARG:NH2	1:A:157:GLU:OE2	2.45	0.43
1:C:164:VAL:HG23	1:E:41:PRO:HD3	2.01	0.43
1:A:20:VAL:HA	1:A:21:PRO:HD3	1.84	0.43
1:E:27:PRO:HB3	1:E:92:ASN:ND2	2.34	0.43
1:B:27:PRO:HD3	1:B:92:ASN:HB3	2.00	0.43
1:D:99:ALA:O	1:D:103:ASN:ND2	2.36	0.43
1:C:114:LEU:HD13	1:C:256:LEU:HD13	2.00	0.43
1:E:20:VAL:HA	1:E:21:PRO:HD3	1.91	0.43
1:E:119:GLY:HA2	1:E:225:LEU:HD11	2.00	0.43
1:H:38:GLN:CD	1:H:245:GLN:HB2	2.43	0.42
1:H:75:VAL:O	1:H:79:LEU:HG	2.19	0.42
1:F:166:LYS:HA	1:F:169:PHE:CE1	2.54	0.42
1:G:144:GLY:HA2	1:G:147:GLU:HG3	2.01	0.42
1:H:199:LEU:HD23	1:H:202:ILE:HD12	2.01	0.42
1:A:112:GLY:HA3	1:A:259:PHE:CZ	2.54	0.42
1:F:62:PRO:O	1:F:66:TYR:OH	2.33	0.42
1:G:52:ASP:OD2	1:G:58:ARG:NH1	2.53	0.42
1:A:177:LYS:HA	1:A:177:LYS:HD2	1.81	0.42
1:C:132:ALA:HA	1:C:135:GLN:HB2	2.00	0.42
1:H:55:GLY:HA2	1:H:61:LYS:HG2	2.02	0.42
1:H:197:ASP:HB3	1:H:198:ARG:HG3	2.02	0.42
1:A:93:SER:HB2	1:A:242:HIS:NE2	2.35	0.42
1:B:4:VAL:HG13	1:B:13:TYR:CE1	2.53	0.42
1:B:200:SER:HA	1:B:230:PRO:HD3	2.01	0.42
1:C:20:VAL:HA	1:C:21:PRO:HD3	1.70	0.42
1:G:194:ASN:OD1	1:G:196:LYS:HG3	2.20	0.42
1:H:127:PRO:HA	1:H:128:PRO:HD3	1.93	0.42
1:C:196:LYS:HG2	1:C:224:LEU:HD21	2.02	0.41
1:G:64:THR:HA	1:G:65:GLY:HA2	1.83	0.41
1:H:27:PRO:HD3	1:H:92:ASN:HB3	2.01	0.41
1:C:167:ALA:HA	1:E:44:GLN:OE1	2.21	0.41
1:H:64:THR:HA	1:H:65:GLY:HA2	1.89	0.41
1:E:9:VAL:HG21	1:E:54:ARG:NH1	2.35	0.41
1:G:244:TYR:OH	1:G:251:GLU:HB3	2.19	0.41
1:H:93:SER:HB2	1:H:242:HIS:NE2	2.35	0.41
1:B:127:PRO:HA	1:B:128:PRO:HD3	1.90	0.41
1:D:29:SER:HA	1:D:175:PHE:CD1	2.56	0.41
1:H:54:ARG:NE	1:H:74:ASP:OD2	2.48	0.41
1:B:171:VAL:HA	1:B:172:PRO:HD2	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ARG:HG3	1:E:66:TYR:CE2	2.56	0.41
1:G:217:THR:HG22	1:G:222:ASN:HD21	1.85	0.41
1:A:11:ILE:HG13	1:A:74:ASP:HB3	2.03	0.41
1:B:108:GLN:CD	1:B:108:GLN:H	2.28	0.41
1:C:58:ARG:HD3	1:E:12:TYR:OH	2.20	0.41
1:C:142:PHE:HB3	1:C:169:PHE:CE2	2.56	0.41
1:D:92:ASN:HA	1:D:116:LEU:O	2.20	0.41
1:E:93:SER:HB2	1:E:242:HIS:NE2	2.35	0.41
1:E:152:ALA:O	1:E:156:ARG:HG3	2.20	0.41
1:E:114:LEU:HD13	1:E:256:LEU:HD13	2.03	0.41
1:B:12:TYR:OH	1:D:58:ARG:HD3	2.22	0.40
1:E:229:ILE:HA	1:E:230:PRO:HD3	1.95	0.40
1:G:142:PHE:HB3	1:G:169:PHE:CZ	2.56	0.40
1:C:117:SER:C	1:C:217:THR:HG21	2.45	0.40
1:D:12:TYR:CD2	1:D:58:ARG:HD2	2.57	0.40
1:G:162:LEU:HG	1:G:166:LYS:HE2	2.03	0.40
1:H:92:ASN:ND2	1:H:116:LEU:O	2.46	0.40
1:B:12:TYR:CD1	1:B:58:ARG:HD2	2.56	0.40
1:F:67:SER:OG	1:F:70:GLU:HG3	2.21	0.40
1:B:72:ALA:HB1	1:B:102:LEU:HD13	2.04	0.40
1:B:58:ARG:HD3	1:D:12:TYR:OH	2.22	0.40
1:C:18:GLU:HA	1:C:19:GLY:HA2	1.82	0.40

All (1) 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)
1:D:64:THR:OG1	1:D:238:ASN:ND2[2_547]	2.15	0.05

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	258/271 (95%)	248 (96%)	10 (4%)	0	100	100
1	B	258/271 (95%)	250 (97%)	7 (3%)	1 (0%)	30	42
1	C	257/271 (95%)	245 (95%)	11 (4%)	1 (0%)	30	42
1	D	257/271 (95%)	249 (97%)	8 (3%)	0	100	100
1	E	257/271 (95%)	250 (97%)	7 (3%)	0	100	100
1	F	258/271 (95%)	251 (97%)	7 (3%)	0	100	100
1	G	257/271 (95%)	250 (97%)	7 (3%)	0	100	100
1	H	256/271 (94%)	243 (95%)	12 (5%)	1 (0%)	30	42
All	All	2058/2168 (95%)	1986 (96%)	69 (3%)	3 (0%)	48	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	197	ASP
1	B	260	VAL
1	C	135	GLN

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	207/218 (95%)	201 (97%)	6 (3%)	37	57
1	B	209/218 (96%)	203 (97%)	6 (3%)	37	57
1	C	209/218 (96%)	204 (98%)	5 (2%)	43	64
1	D	208/218 (95%)	204 (98%)	4 (2%)	50	70
1	E	208/218 (95%)	205 (99%)	3 (1%)	59	75
1	F	206/218 (94%)	200 (97%)	6 (3%)	37	57
1	G	200/218 (92%)	196 (98%)	4 (2%)	48	68
1	H	198/218 (91%)	193 (98%)	5 (2%)	42	63
All	All	1645/1744 (94%)	1606 (98%)	39 (2%)	43	64

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	6	ASN
1	A	50	VAL
1	A	146	LEU
1	A	217	THR
1	A	238	ASN
1	B	76	VAL
1	B	219	VAL
1	B	238	ASN
1	B	239	ASP
1	B	240	VAL
1	B	254	GLU
1	C	20	VAL
1	C	109	ARG
1	C	217	THR
1	C	235	ARG
1	C	238	ASN
1	D	69	MET
1	D	86	ARG
1	D	104	LEU
1	D	129	GLU
1	E	44	GLN
1	E	64	THR
1	E	92	ASN
1	F	4	VAL
1	F	50	VAL
1	F	76	VAL
1	F	190	VAL
1	F	254	GLU
1	F	260	VAL
1	G	94	ILE
1	G	108	GLN
1	G	197	ASP
1	G	217	THR
1	H	50	VAL
1	H	64	THR
1	H	69	MET
1	H	190	VAL
1	H	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	B	44	GLN
1	B	46	ASN
1	B	103	ASN
1	B	113	ASN
1	B	222	ASN
1	C	38	GLN
1	C	92	ASN
1	D	44	GLN
1	D	46	ASN
1	E	135	GLN
1	F	92	ASN
1	G	238	ASN
1	H	103	ASN
1	H	113	ASN
1	H	223	GLN

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 ⓘ

There are no ligands in this entry.

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	260/271 (95%)	0.38	7 (2%) 56 51	20, 30, 48, 63	0
1	B	260/271 (95%)	0.16	5 (1%) 66 62	18, 25, 39, 67	0
1	C	259/271 (95%)	0.20	5 (1%) 66 62	19, 25, 44, 66	0
1	D	259/271 (95%)	0.19	5 (1%) 66 62	18, 26, 46, 69	0
1	E	259/271 (95%)	0.17	6 (2%) 61 57	18, 24, 45, 65	0
1	F	260/271 (95%)	0.21	5 (1%) 66 62	20, 26, 43, 63	0
1	G	259/271 (95%)	1.06	30 (11%) 9 7	27, 44, 67, 73	0
1	H	258/271 (95%)	0.84	26 (10%) 12 10	25, 39, 55, 66	0
All	All	2074/2168 (95%)	0.40	89 (4%) 40 33	18, 28, 55, 73	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	ARG	4.8
1	D	260	VAL	4.4
1	A	259	PHE	4.1
1	G	185	ALA	4.1
1	E	259	PHE	4.1
1	E	130	ALA	3.5
1	E	260	VAL	3.4
1	G	260	VAL	3.3
1	H	255	LEU	3.3
1	C	259	PHE	3.2
1	F	261	ALA	3.2
1	H	3	HIS	3.1
1	B	261	ALA	3.1
1	B	260	VAL	3.0
1	G	190	VAL	3.0
1	B	259	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	183	ALA	2.9
1	H	199	LEU	2.9
1	H	93	SER	2.9
1	G	93	SER	2.8
1	A	138	TYR	2.8
1	G	138	TYR	2.8
1	G	188	ASN	2.8
1	C	136	ASN	2.8
1	G	172	PRO	2.8
1	H	128	PRO	2.8
1	G	60	ASP	2.8
1	H	228	ASN	2.7
1	A	260	VAL	2.7
1	G	180	PHE	2.7
1	G	259	PHE	2.7
1	H	197	ASP	2.7
1	G	66	TYR	2.7
1	G	192	ALA	2.7
1	G	131	GLY	2.7
1	A	261	ALA	2.6
1	G	173	SER	2.6
1	H	114	LEU	2.6
1	H	153	ARG	2.6
1	G	81	ALA	2.6
1	G	202	ILE	2.5
1	F	129	GLU	2.5
1	F	125	GLY	2.5
1	D	108	GLN	2.5
1	G	139	ILE	2.5
1	G	197	ASP	2.5
1	H	17	GLY	2.5
1	H	223	GLN	2.5
1	C	257	ARG	2.5
1	C	260	VAL	2.5
1	E	64	THR	2.4
1	H	117	SER	2.4
1	A	142	PHE	2.4
1	E	93	SER	2.4
1	H	230	PRO	2.4
1	G	55	GLY	2.4
1	H	219	VAL	2.4
1	B	97	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	125	GLY	2.3
1	G	179	VAL	2.3
1	H	152	ALA	2.3
1	H	104	LEU	2.3
1	G	94	ILE	2.3
1	H	200	SER	2.3
1	E	108	GLN	2.3
1	H	233	GLU	2.3
1	G	136	ASN	2.3
1	H	229	ILE	2.2
1	H	205	PRO	2.2
1	H	79	LEU	2.2
1	G	119	GLY	2.2
1	H	102	LEU	2.2
1	H	259	PHE	2.2
1	G	130	ALA	2.2
1	G	135	GLN	2.2
1	D	136	ASN	2.1
1	F	93	SER	2.1
1	H	202	ILE	2.1
1	H	204	ALA	2.1
1	F	257	ARG	2.1
1	G	73	ASP	2.1
1	G	141	ALA	2.1
1	D	129	GLU	2.1
1	H	135	GLN	2.1
1	C	212	GLU	2.1
1	D	130	ALA	2.1
1	A	8	GLY	2.1
1	B	129	GLU	2.0
1	A	203	GLN	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 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.