Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 01:11 PM JST

PDB ID	:	5EGN
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:

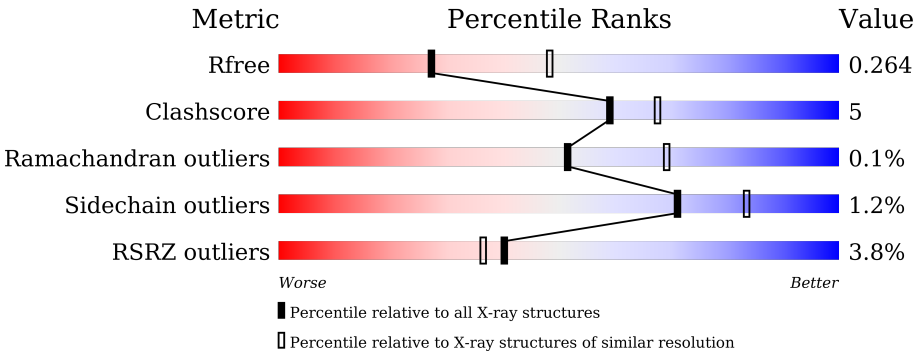
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (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 <=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	3% 85% 11%
1	B	271	% 83% 12%
1	C	271	2% 83% 12%
1	D	271	2% 85% 10%
1	E	271	3% 82% 13%
1	F	271	2% 86% 10%

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Mol	Chain	Length	Quality of chain
1	G	271	11% 83% 13% •
1	H	271	5% 81% 14% • 5%

2 Entry composition (i)

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

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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

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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.

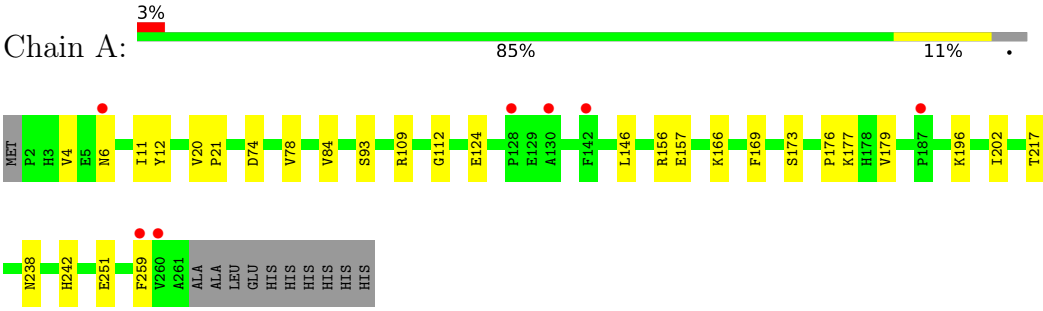
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	41	Total O 41 41	0	0
2	B	67	Total O 67 67	0	0
2	C	59	Total O 59 59	0	0
2	D	49	Total O 49 49	0	0
2	E	58	Total O 58 58	0	0
2	F	61	Total O 61 61	0	0
2	G	28	Total O 28 28	0	0
2	H	37	Total O 37 37	0	0

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.

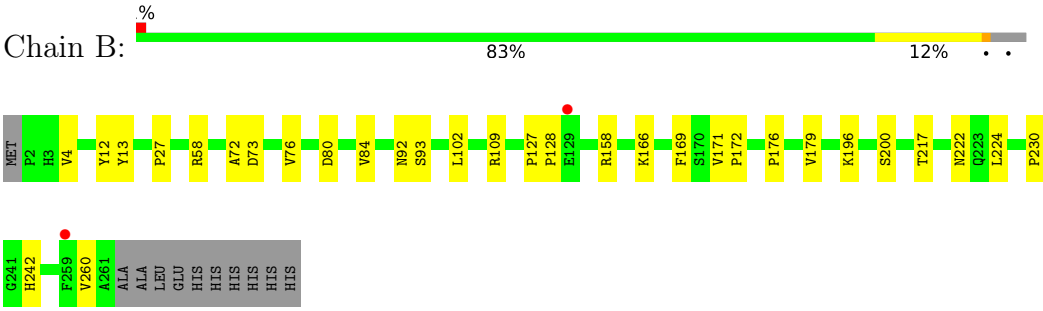
• Molecule 1: Esterase

Chain A:



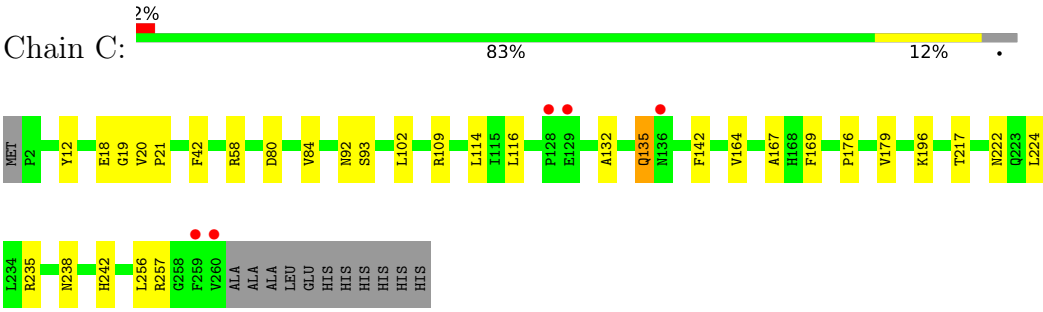
• Molecule 1: Esterase

Chain B:



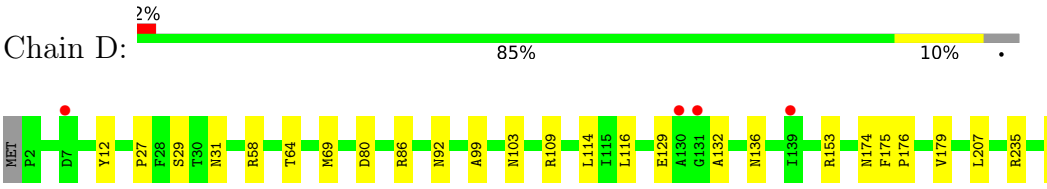
• Molecule 1: Esterase

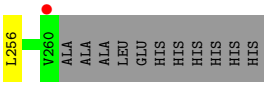
Chain C:



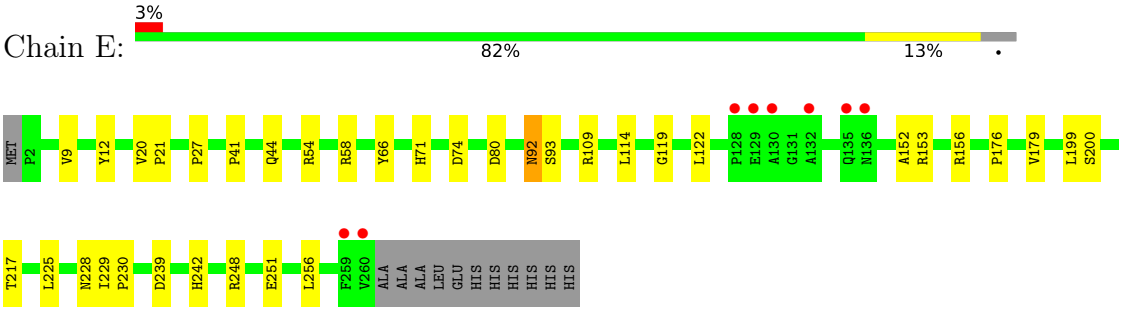
• Molecule 1: Esterase

Chain D:

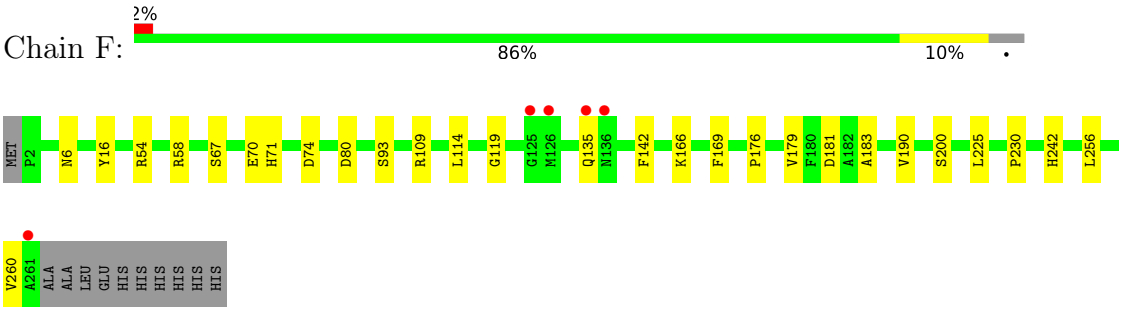




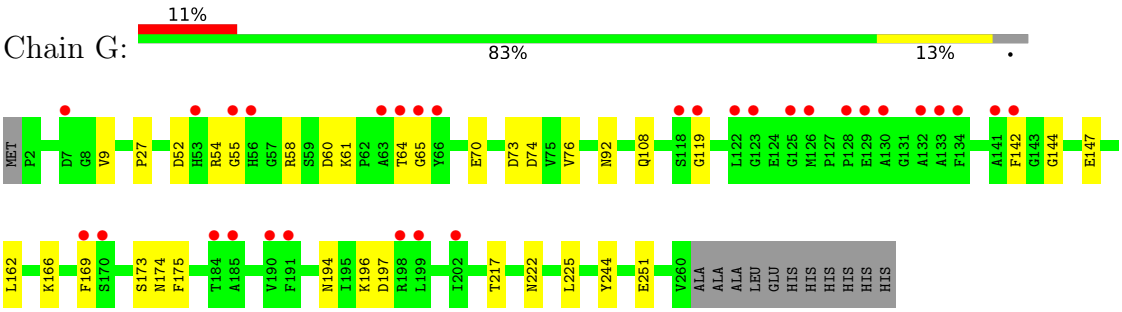
• Molecule 1: Esterase



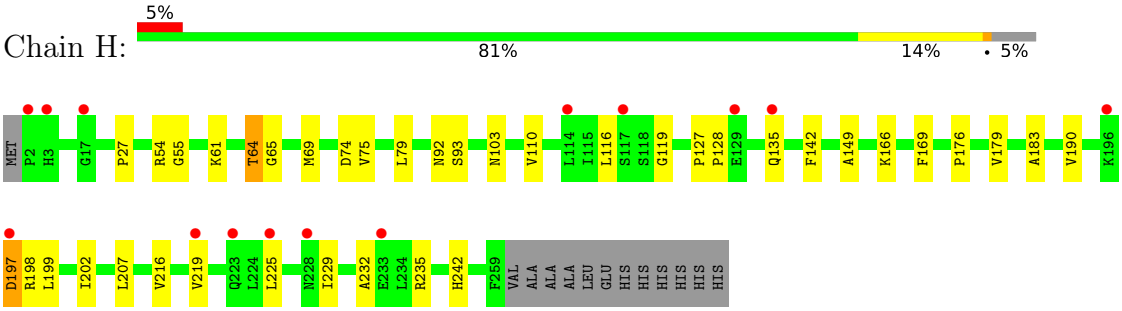
• Molecule 1: Esterase



• Molecule 1: Esterase



• Molecule 1: Esterase



4 Data and refinement statistics (i)

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) 91.2 (44.82-2.64)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.219 , 0.264 0.223 , 0.264	Depositor DCC
R_{free} test set	2981 reflections (5.20%)	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)	0.35 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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

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	0.23	0/2033	0.40	0/2767
1	B	0.23	0/2041	0.40	0/2777
1	C	0.23	0/2036	0.41	0/2770
1	D	0.23	0/2029	0.40	0/2761
1	E	0.23	0/2029	0.41	0/2761
1	F	0.24	0/2027	0.42	0/2758
1	G	0.24	0/1997	0.42	0/2720
1	H	0.25	0/1983	0.43	0/2703
All	All	0.24	0/16175	0.41	0/22017

There are no bond length outliers.

There are no bond angle outliers.

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	22	0
1	C	1986	0	1926	18	0
1	D	1980	0	1919	17	1
1	E	1980	0	1919	26	0
1	F	1979	0	1914	14	0
1	G	1950	0	1860	21	0
1	H	1935	0	1849	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	146	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 (146) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:54:ARG:HE	1:G:74:ASP:CG	2.12	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:58:ARG:NH2	2:B:309:HOH:O	2.50	0.44
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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%)	34	48
1	C	257/271 (95%)	245 (95%)	11 (4%)	1 (0%)	34	48
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%)	34	48
All	All	2058/2168 (95%)	1986 (96%)	69 (3%)	3 (0%)	51	69

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 (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	207/218 (95%)	204 (99%)	3 (1%)	67	80
1	B	209/218 (96%)	206 (99%)	3 (1%)	67	80
1	C	209/218 (96%)	207 (99%)	2 (1%)	76	86
1	D	208/218 (95%)	205 (99%)	3 (1%)	67	80
1	E	208/218 (95%)	207 (100%)	1 (0%)	88	94
1	F	206/218 (94%)	203 (98%)	3 (2%)	65	79
1	G	200/218 (92%)	198 (99%)	2 (1%)	76	86
1	H	198/218 (91%)	195 (98%)	3 (2%)	65	79
All	All	1645/1744 (94%)	1625 (99%)	20 (1%)	71	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	146	LEU
1	A	238	ASN
1	B	238	ASN
1	B	239	ASP
1	B	240	VAL
1	C	102	LEU
1	C	238	ASN
1	D	69	MET
1	D	86	ARG
1	D	129	GLU
1	E	92	ASN
1	F	6	ASN
1	F	142	PHE
1	F	260	VAL
1	G	108	GLN
1	G	197	ASP
1	H	64	THR
1	H	142	PHE
1	H	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	ASN

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

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, 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	260/271 (95%)	0.11	7 (2%) 54 50	20, 30, 48, 63	0
1	B	260/271 (95%)	-0.14	2 (0%) 86 85	18, 25, 39, 67	0
1	C	259/271 (95%)	-0.11	6 (2%) 60 57	19, 25, 44, 66	0
1	D	259/271 (95%)	-0.05	5 (1%) 66 64	18, 26, 46, 69	0
1	E	259/271 (95%)	-0.06	8 (3%) 49 45	18, 24, 45, 65	0
1	F	260/271 (95%)	-0.10	5 (1%) 66 64	20, 26, 43, 63	0
1	G	259/271 (95%)	0.73	31 (11%) 4 3	27, 44, 67, 73	0
1	H	258/271 (95%)	0.45	14 (5%) 25 22	25, 39, 55, 66	0
All	All	2074/2168 (95%)	0.10	78 (3%) 40 36	18, 28, 55, 73	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	130	ALA	5.3
1	G	130	ALA	5.2
1	G	66	TYR	5.0
1	G	185	ALA	4.8
1	D	130	ALA	4.3
1	A	259	PHE	4.2
1	F	125	GLY	3.9
1	C	128	PRO	3.7
1	C	129	GLU	3.6
1	H	197	ASP	3.6
1	E	128	PRO	3.5
1	G	132	ALA	3.4
1	G	190	VAL	3.4
1	G	141	ALA	3.4
1	G	128	PRO	3.4
1	G	125	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	17	GLY	3.2
1	G	198	ARG	3.2
1	G	119	GLY	3.0
1	E	132	ALA	3.0
1	G	191	PHE	2.9
1	G	129	GLU	2.9
1	A	6	ASN	2.9
1	G	118	SER	2.9
1	A	260	VAL	2.8
1	H	3	HIS	2.8
1	D	260	VAL	2.7
1	E	129	GLU	2.7
1	G	142	PHE	2.7
1	G	133	ALA	2.7
1	G	170	SER	2.7
1	G	134	PHE	2.7
1	G	126	MET	2.6
1	E	136	ASN	2.6
1	G	55	GLY	2.6
1	D	139	ILE	2.5
1	A	130	ALA	2.5
1	B	259	PHE	2.5
1	H	233	GLU	2.4
1	G	7	ASP	2.4
1	G	202	ILE	2.4
1	F	136	ASN	2.4
1	F	261	ALA	2.4
1	H	129	GLU	2.4
1	D	131	GLY	2.3
1	G	63	ALA	2.3
1	H	135	GLN	2.3
1	G	199	LEU	2.3
1	G	169	PHE	2.3
1	E	260	VAL	2.3
1	A	187	PRO	2.3
1	E	135	GLN	2.3
1	B	129	GLU	2.3
1	H	117	SER	2.2
1	G	122	LEU	2.2
1	C	259	PHE	2.2
1	H	223	GLN	2.2
1	G	184	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	PHE	2.2
1	F	135	GLN	2.2
1	C	260	VAL	2.2
1	C	136	ASN	2.2
1	G	56	HIS	2.1
1	A	128	PRO	2.1
1	H	2	PRO	2.1
1	D	7	ASP	2.1
1	F	126	MET	2.1
1	H	196	LYS	2.1
1	G	65	GLY	2.1
1	G	53	HIS	2.1
1	H	225	LEU	2.1
1	E	259	PHE	2.1
1	G	123	GLY	2.1
1	H	228	ASN	2.0
1	H	114	LEU	2.0
1	C	227	ASP	2.0
1	H	219	VAL	2.0
1	G	64	THR	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 monosaccharides 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.