



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:19 PM GMT

PDB ID : 2Q17
Title : Formylglycine Generating Enzyme from Streptomyces coelicolor
Authors : Carlson, B.L.; Ballister, E.R.; Skordalakes, E.; King, D.S.; Breidenbach, M.A.;
Gilmore, S.A.; Berger, J.M.; Bertozzi, C.R.
Deposited on : 2007-05-23
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

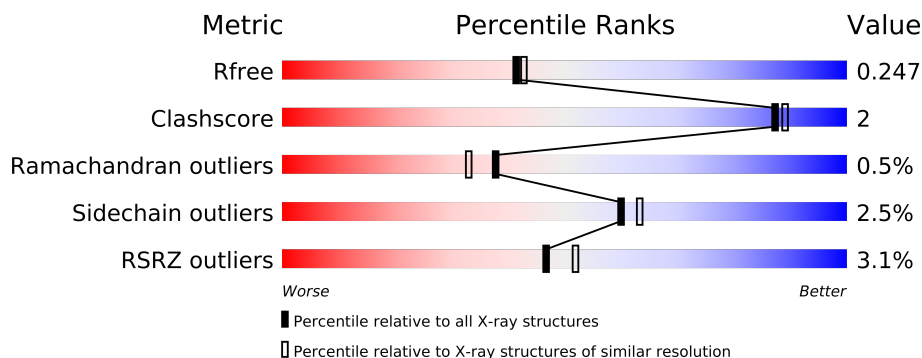
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	346	
1	B	346	
1	C	346	
1	D	346	
1	E	346	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12171 atoms, of which 0 are hydrogen and 0 are deuterium.

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 formylglycine generating enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	2	0
			2240	1396	429	407	8			
1	B	288	Total	C	N	O	S	0	2	0
			2243	1397	429	409	8			
1	C	287	Total	C	N	O	S	0	2	0
			2232	1391	425	408	8			
1	D	286	Total	C	N	O	S	0	2	0
			2224	1387	424	405	8			
1	E	289	Total	C	N	O	S	0	2	0
			2251	1403	430	410	8			

There are 170 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
A	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
A	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
A	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
A	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
A	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
A	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
A	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
A	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
A	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
A	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
A	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
A	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
A	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
A	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
A	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
A	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
A	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
A	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
A	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
A	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
A	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
B	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
B	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
B	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
B	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
B	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
B	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
B	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
B	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
B	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
B	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
B	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
B	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
B	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
B	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
B	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
B	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
B	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
B	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
B	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
B	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
B	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
B	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
C	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
C	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
C	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
C	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
C	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
C	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
C	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
C	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
C	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
C	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
C	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
C	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
C	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
C	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
C	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
C	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
C	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
C	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
C	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
C	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
C	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
C	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
C	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
D	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
D	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
D	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7
D	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
D	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
D	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
D	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
D	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
D	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
D	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
D	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
D	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
D	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
D	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
D	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
D	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
D	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
D	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
D	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
D	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
D	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
D	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
E	-31	MET	-	EXPRESSION TAG	UNP Q9F3C7
E	-30	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-29	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-28	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-27	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-26	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-25	HIS	-	EXPRESSION TAG	UNP Q9F3C7
E	-24	GLY	-	EXPRESSION TAG	UNP Q9F3C7
E	-23	LYS	-	EXPRESSION TAG	UNP Q9F3C7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	-21	ILE	-	EXPRESSION TAG	UNP Q9F3C7
E	-20	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	-19	ASN	-	EXPRESSION TAG	UNP Q9F3C7
E	-18	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	-17	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-16	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-15	GLY	-	EXPRESSION TAG	UNP Q9F3C7
E	-14	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-13	ASP	-	EXPRESSION TAG	UNP Q9F3C7
E	-12	SER	-	EXPRESSION TAG	UNP Q9F3C7
E	-11	THR	-	EXPRESSION TAG	UNP Q9F3C7
E	-10	GLU	-	EXPRESSION TAG	UNP Q9F3C7
E	-9	ASN	-	EXPRESSION TAG	UNP Q9F3C7
E	-8	LEU	-	EXPRESSION TAG	UNP Q9F3C7
E	-7	TYR	-	EXPRESSION TAG	UNP Q9F3C7
E	-6	PHE	-	EXPRESSION TAG	UNP Q9F3C7
E	-5	GLN	-	EXPRESSION TAG	UNP Q9F3C7
E	-4	GLY	-	EXPRESSION TAG	UNP Q9F3C7
E	-3	ILE	-	EXPRESSION TAG	UNP Q9F3C7
E	-2	ASP	-	EXPRESSION TAG	UNP Q9F3C7
E	-1	PRO	-	EXPRESSION TAG	UNP Q9F3C7
E	0	PHE	-	EXPRESSION TAG	UNP Q9F3C7
E	1	THR	-	EXPRESSION TAG	UNP Q9F3C7
E	2	ASP	-	EXPRESSION TAG	UNP Q9F3C7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

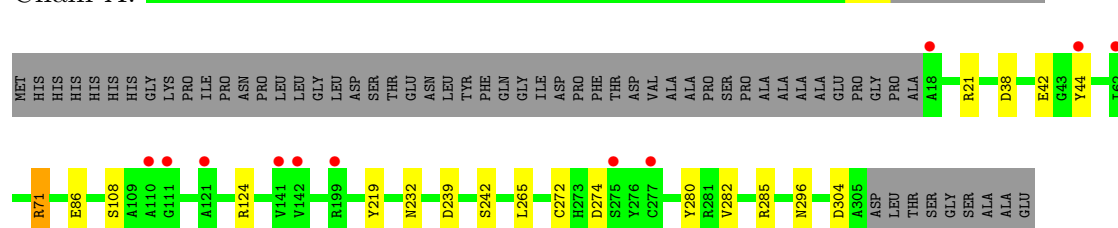
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total 210	O 210	0	0
3	B	195	Total 195	O 195	0	0
3	C	170	Total 170	O 170	0	0
3	D	189	Total 189	O 189	0	0
3	E	212	Total 212	O 212	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

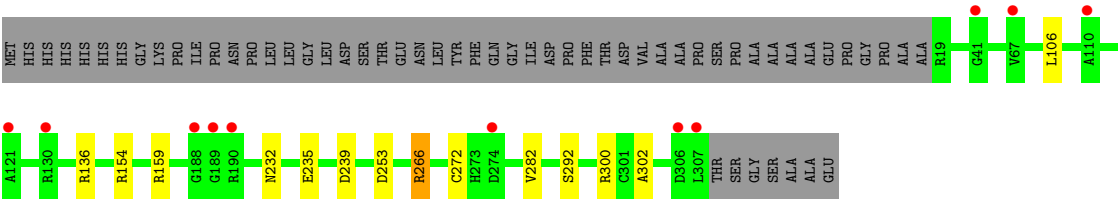
- Molecule 1: formylglycine generating enzyme

Chain A:



● Molecule 1: formylglycine generating enzyme

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.44Å 142.44Å 217.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 17.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-2.10) 84.3 (17.40-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.241 0.209 , 0.247	Depositor DCC
R_{free} test set	7861 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 155975 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12171	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8857e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.44	0/2317	0.57	0/3166
1	B	0.45	0/2320	0.56	1/3170 (0.0%)
1	C	0.42	0/2309	0.55	0/3155
1	D	0.44	0/2301	0.56	0/3144
1	E	0.44	0/2328	0.59	2/3181 (0.1%)
All	All	0.44	0/11575	0.57	3/15816 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	266	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	E	266	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	266	ARG	NE-CZ-NH2	-5.31	117.64	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2240	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2243	0	0	4	0
1	C	2232	0	0	5	0
1	D	2224	0	0	6	0
1	E	2251	0	0	7	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
3	A	210	0	0	1	0
3	B	195	0	0	2	0
3	C	170	0	0	3	0
3	D	189	0	0	3	0
3	E	212	0	0	4	0
All	All	12171	0	0	28	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (28) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:272[A]:CYS:SG	3:E:513:HOH:O	2.32	0.86
1:C:285:ARG:NH1	3:C:466:HOH:O	2.21	0.72
1:E:136:ARG:NH1	3:E:501:HOH:O	2.23	0.72
1:D:242:SER:O	1:D:285:ARG:NH2	2.28	0.66
1:A:242:SER:O	1:A:285:ARG:NH2	2.30	0.64
1:C:285:ARG:NH2	3:C:466:HOH:O	2.35	0.59
1:D:253:ASP:CB	3:D:498:HOH:O	2.52	0.56
1:C:272[A]:CYS:SG	3:C:469:HOH:O	2.59	0.52
1:B:158:LYS:NZ	3:B:504:HOH:O	2.44	0.50
1:D:199:ARG:NH1	3:D:454:HOH:O	2.44	0.50
1:A:71:ARG:NH1	3:A:523:HOH:O	2.44	0.49
1:D:132:ASP:O	1:D:136:ARG:NH2	2.46	0.48
1:E:154:ARG:NH2	3:E:523:HOH:O	2.48	0.47
1:C:21:ARG:NH2	1:C:304:ASP:O	2.48	0.47
1:A:21:ARG:NH1	1:A:304:ASP:O	2.49	0.46
1:E:235:GLU:OE1	1:E:300:ARG:NE	2.49	0.46
1:D:266:ARG:NH2	1:D:282:VAL:O	2.49	0.45
1:B:27:VAL:CG2	3:B:496:HOH:O	2.64	0.45
1:E:253:ASP:CB	3:E:522:HOH:O	2.64	0.45
1:A:86:GLU:OE1	1:A:124:ARG:NH2	2.50	0.45
1:E:266:ARG:NH2	1:E:282:VAL:O	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:163:GLU:OE2	1:B:285:ARG:NE	2.52	0.43
1:D:202:HIS:CD2	3:D:405:HOH:O	2.72	0.42
1:A:38:ASP:OD2	1:A:42:GLU:N	2.52	0.42
1:A:272[B]:CYS:SG	1:A:280:TYR:CD2	3.13	0.42
1:B:269:SER:N	1:B:272[A]:CYS:SG	2.93	0.42
1:C:266:ARG:NH2	1:C:282:VAL:O	2.54	0.41
1:E:159:ARG:O	1:E:302:ALA:N	2.54	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/346 (83%)	277 (96%)	9 (3%)	2 (1%)	30	23
1	B	288/346 (83%)	279 (97%)	8 (3%)	1 (0%)	50	49
1	C	287/346 (83%)	276 (96%)	9 (3%)	2 (1%)	30	23
1	D	286/346 (83%)	273 (96%)	12 (4%)	1 (0%)	50	49
1	E	289/346 (84%)	279 (96%)	9 (3%)	1 (0%)	50	49
All	All	1438/1730 (83%)	1384 (96%)	47 (3%)	7 (0%)	38	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	219	TYR
1	A	219	TYR
1	A	232	ASN
1	B	232	ASN
1	C	232	ASN
1	D	232	ASN
1	E	232	ASN

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	219/261 (84%)	211 (96%)	8 (4%)	45	45
1	B	220/261 (84%)	213 (97%)	7 (3%)	51	52
1	C	219/261 (84%)	213 (97%)	6 (3%)	57	60
1	D	218/261 (84%)	215 (99%)	3 (1%)	78	83
1	E	221/261 (85%)	218 (99%)	3 (1%)	78	83
All	All	1097/1305 (84%)	1070 (98%)	27 (2%)	60	63

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TYR
1	A	71	ARG
1	A	108	SER
1	A	239	ASP
1	A	265	LEU
1	A	274	ASP
1	A	282	VAL
1	A	296	ASN
1	B	57	LEU
1	B	82	VAL
1	B	239	ASP
1	B	251	THR
1	B	265	LEU
1	B	274	ASP
1	B	303	ASN
1	C	57	LEU
1	C	239	ASP
1	C	251	THR
1	C	265	LEU
1	C	285	ARG
1	C	306	ASP
1	D	57	LEU
1	D	211	LEU
1	D	239	ASP
1	E	106	LEU

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Mol	Chain	Res	Type
1	E	239	ASP
1	E	292	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 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.

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	288/346 (83%)	0.17	11 (3%) 38 43	39, 41, 42, 44	0
1	B	288/346 (83%)	0.11	6 (2%) 60 65	40, 41, 42, 44	0
1	C	287/346 (82%)	0.15	10 (3%) 42 46	40, 41, 42, 43	0
1	D	286/346 (82%)	0.11	7 (2%) 56 61	40, 41, 42, 44	0
1	E	289/346 (83%)	0.18	11 (3%) 38 43	40, 41, 42, 44	0
All	All	1438/1730 (83%)	0.14	45 (3%) 47 52	39, 41, 42, 44	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	307	LEU	6.5
1	C	306	ASP	5.0
1	C	20	PRO	3.9
1	B	306	ASP	3.9
1	A	18	ALA	3.4
1	E	110	ALA	3.1
1	B	188	GLY	3.1
1	A	142	VAL	3.0
1	A	110	ALA	2.9
1	B	110	ALA	2.9
1	A	277[A]	CYS	2.8
1	D	190	ARG	2.7
1	E	190	ARG	2.7
1	C	134	THR	2.7
1	D	188	GLY	2.7
1	A	44	TYR	2.7
1	E	306	ASP	2.6
1	D	20	PRO	2.6
1	C	144	VAL	2.6
1	A	111	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	188	GLY	2.5
1	A	141	VAL	2.4
1	E	121	ALA	2.4
1	E	189	GLY	2.4
1	E	41	GLY	2.4
1	D	305	ALA	2.4
1	C	88	PHE	2.3
1	B	275	SER	2.3
1	B	20	PRO	2.3
1	A	275	SER	2.3
1	B	190	ARG	2.2
1	E	274	ASP	2.2
1	C	274	ASP	2.2
1	C	39	ALA	2.1
1	D	144	VAL	2.1
1	E	130	ARG	2.1
1	C	188	GLY	2.1
1	D	67	VAL	2.1
1	C	41	GLY	2.1
1	D	44	TYR	2.1
1	E	67	VAL	2.0
1	A	121	ALA	2.0
1	C	109	ALA	2.0
1	A	62	ILE	2.0
1	A	199	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	315	1/1	0.07	-1.40	34,34,34,34	0
2	CA	E	315	1/1	0.08	-1.53	44,44,44,44	0
2	CA	C	315	1/1	0.04	-2.21	32,32,32,32	0
2	CA	D	315	1/1	0.05	-2.86	28,28,28,28	0
2	CA	B	315	1/1	0.04	-3.61	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.