



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:07 AM UTC

PDB ID : 5BYW / pdb_00005byw
Title : Crystal structure of engineered trifunctional CtCEL5E
Authors : Lin, W.L.; Liang, P.H.; Ho, M.C.
Deposited on : 2015-06-11
Resolution : 2.60 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

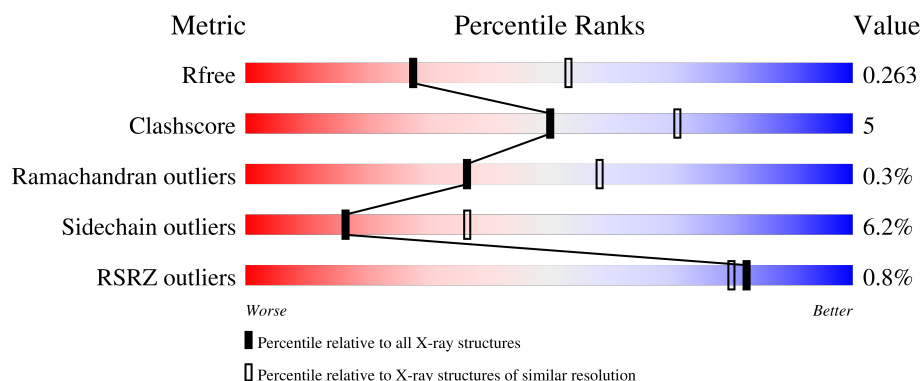
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	414	 67% 9% • 23%
1	B	414	 67% 8% • 24%
1	C	414	 61% 14% • 23%
1	D	414	 63% 11% • 23%
1	E	414	 67% 8% • 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13396 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 Endoglucanase H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2639	1688	442	498	11			
1	B	316	Total	C	N	O	S	0	0	0
			2623	1679	439	494	11			
1	C	318	Total	C	N	O	S	0	0	0
			2634	1685	441	497	11			
1	D	320	Total	C	N	O	S	0	0	0
			2648	1694	444	499	11			
1	E	323	Total	C	N	O	S	0	0	0
			2676	1714	446	505	11			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P16218
A	2	GLY	-	expression tag	UNP P16218
A	3	SER	-	expression tag	UNP P16218
A	4	SER	-	expression tag	UNP P16218
A	5	HIS	-	expression tag	UNP P16218
A	6	HIS	-	expression tag	UNP P16218
A	7	HIS	-	expression tag	UNP P16218
A	8	HIS	-	expression tag	UNP P16218
A	9	HIS	-	expression tag	UNP P16218
A	10	HIS	-	expression tag	UNP P16218
A	11	SER	-	expression tag	UNP P16218
A	12	SER	-	expression tag	UNP P16218
A	13	GLY	-	expression tag	UNP P16218
A	14	LEU	-	expression tag	UNP P16218
A	15	VAL	-	expression tag	UNP P16218
A	16	PRO	-	expression tag	UNP P16218
A	17	ARG	-	expression tag	UNP P16218
A	18	GLY	-	expression tag	UNP P16218
A	19	SER	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	HIS	-	expression tag	UNP P16218
A	21	MET	-	expression tag	UNP P16218
A	22	ALA	-	expression tag	UNP P16218
A	23	SER	-	expression tag	UNP P16218
A	24	MET	-	expression tag	UNP P16218
A	25	THR	-	expression tag	UNP P16218
A	26	GLY	-	expression tag	UNP P16218
A	27	GLY	-	expression tag	UNP P16218
A	28	GLN	-	expression tag	UNP P16218
A	29	GLN	-	expression tag	UNP P16218
A	30	MET	-	expression tag	UNP P16218
A	31	GLY	-	expression tag	UNP P16218
A	32	ARG	-	expression tag	UNP P16218
A	33	ILE	-	expression tag	UNP P16218
A	34	GLU	-	expression tag	UNP P16218
A	35	GLY	-	expression tag	UNP P16218
A	36	ARG	-	expression tag	UNP P16218
A	37	GLU	-	expression tag	UNP P16218
A	38	PHE	-	expression tag	UNP P16218
A	267	ALA	PHE	engineered mutation	UNP P16218
A	273	PHE	TYR	engineered mutation	UNP P16218
A	278	GLN	-	insertion	UNP P16218
A	279	GLY	-	insertion	UNP P16218
A	280	ALA	-	insertion	UNP P16218
A	281	GLU	-	insertion	UNP P16218
A	282	TRP	-	insertion	UNP P16218
A	283	VAL	-	insertion	UNP P16218
A	284	GLU	-	insertion	UNP P16218
A	285	GLY	-	insertion	UNP P16218
A	286	SER	-	insertion	UNP P16218
A	287	GLU	-	insertion	UNP P16218
A	288	LYS	-	insertion	UNP P16218
A	289	TRP	LYS	engineered mutation	UNP P16218
A	290	LEU	TRP	engineered mutation	UNP P16218
A	291	GLY	ARG	engineered mutation	UNP P16218
A	292	ARG	GLY	engineered mutation	UNP P16218
A	293	LYS	THR	engineered mutation	UNP P16218
B	1	MET	-	initiating methionine	UNP P16218
B	2	GLY	-	expression tag	UNP P16218
B	3	SER	-	expression tag	UNP P16218
B	4	SER	-	expression tag	UNP P16218
B	5	HIS	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP P16218
B	7	HIS	-	expression tag	UNP P16218
B	8	HIS	-	expression tag	UNP P16218
B	9	HIS	-	expression tag	UNP P16218
B	10	HIS	-	expression tag	UNP P16218
B	11	SER	-	expression tag	UNP P16218
B	12	SER	-	expression tag	UNP P16218
B	13	GLY	-	expression tag	UNP P16218
B	14	LEU	-	expression tag	UNP P16218
B	15	VAL	-	expression tag	UNP P16218
B	16	PRO	-	expression tag	UNP P16218
B	17	ARG	-	expression tag	UNP P16218
B	18	GLY	-	expression tag	UNP P16218
B	19	SER	-	expression tag	UNP P16218
B	20	HIS	-	expression tag	UNP P16218
B	21	MET	-	expression tag	UNP P16218
B	22	ALA	-	expression tag	UNP P16218
B	23	SER	-	expression tag	UNP P16218
B	24	MET	-	expression tag	UNP P16218
B	25	THR	-	expression tag	UNP P16218
B	26	GLY	-	expression tag	UNP P16218
B	27	GLY	-	expression tag	UNP P16218
B	28	GLN	-	expression tag	UNP P16218
B	29	GLN	-	expression tag	UNP P16218
B	30	MET	-	expression tag	UNP P16218
B	31	GLY	-	expression tag	UNP P16218
B	32	ARG	-	expression tag	UNP P16218
B	33	ILE	-	expression tag	UNP P16218
B	34	GLU	-	expression tag	UNP P16218
B	35	GLY	-	expression tag	UNP P16218
B	36	ARG	-	expression tag	UNP P16218
B	37	GLU	-	expression tag	UNP P16218
B	38	PHE	-	expression tag	UNP P16218
B	267	ALA	PHE	engineered mutation	UNP P16218
B	273	PHE	TYR	engineered mutation	UNP P16218
B	278	GLN	-	insertion	UNP P16218
B	279	GLY	-	insertion	UNP P16218
B	280	ALA	-	insertion	UNP P16218
B	281	GLU	-	insertion	UNP P16218
B	282	TRP	-	insertion	UNP P16218
B	283	VAL	-	insertion	UNP P16218
B	284	GLU	-	insertion	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
B	285	GLY	-	insertion	UNP P16218
B	286	SER	-	insertion	UNP P16218
B	287	GLU	-	insertion	UNP P16218
B	288	LYS	-	insertion	UNP P16218
B	289	TRP	LYS	engineered mutation	UNP P16218
B	290	LEU	TRP	engineered mutation	UNP P16218
B	291	GLY	ARG	engineered mutation	UNP P16218
B	292	ARG	GLY	engineered mutation	UNP P16218
B	293	LYS	THR	engineered mutation	UNP P16218
C	1	MET	-	initiating methionine	UNP P16218
C	2	GLY	-	expression tag	UNP P16218
C	3	SER	-	expression tag	UNP P16218
C	4	SER	-	expression tag	UNP P16218
C	5	HIS	-	expression tag	UNP P16218
C	6	HIS	-	expression tag	UNP P16218
C	7	HIS	-	expression tag	UNP P16218
C	8	HIS	-	expression tag	UNP P16218
C	9	HIS	-	expression tag	UNP P16218
C	10	HIS	-	expression tag	UNP P16218
C	11	SER	-	expression tag	UNP P16218
C	12	SER	-	expression tag	UNP P16218
C	13	GLY	-	expression tag	UNP P16218
C	14	LEU	-	expression tag	UNP P16218
C	15	VAL	-	expression tag	UNP P16218
C	16	PRO	-	expression tag	UNP P16218
C	17	ARG	-	expression tag	UNP P16218
C	18	GLY	-	expression tag	UNP P16218
C	19	SER	-	expression tag	UNP P16218
C	20	HIS	-	expression tag	UNP P16218
C	21	MET	-	expression tag	UNP P16218
C	22	ALA	-	expression tag	UNP P16218
C	23	SER	-	expression tag	UNP P16218
C	24	MET	-	expression tag	UNP P16218
C	25	THR	-	expression tag	UNP P16218
C	26	GLY	-	expression tag	UNP P16218
C	27	GLY	-	expression tag	UNP P16218
C	28	GLN	-	expression tag	UNP P16218
C	29	GLN	-	expression tag	UNP P16218
C	30	MET	-	expression tag	UNP P16218
C	31	GLY	-	expression tag	UNP P16218
C	32	ARG	-	expression tag	UNP P16218
C	33	ILE	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
C	34	GLU	-	expression tag	UNP P16218
C	35	GLY	-	expression tag	UNP P16218
C	36	ARG	-	expression tag	UNP P16218
C	37	GLU	-	expression tag	UNP P16218
C	38	PHE	-	expression tag	UNP P16218
C	267	ALA	PHE	engineered mutation	UNP P16218
C	273	PHE	TYR	engineered mutation	UNP P16218
C	278	GLN	-	insertion	UNP P16218
C	279	GLY	-	insertion	UNP P16218
C	280	ALA	-	insertion	UNP P16218
C	281	GLU	-	insertion	UNP P16218
C	282	TRP	-	insertion	UNP P16218
C	283	VAL	-	insertion	UNP P16218
C	284	GLU	-	insertion	UNP P16218
C	285	GLY	-	insertion	UNP P16218
C	286	SER	-	insertion	UNP P16218
C	287	GLU	-	insertion	UNP P16218
C	288	LYS	-	insertion	UNP P16218
C	289	TRP	LYS	engineered mutation	UNP P16218
C	290	LEU	TRP	engineered mutation	UNP P16218
C	291	GLY	ARG	engineered mutation	UNP P16218
C	292	ARG	GLY	engineered mutation	UNP P16218
C	293	LYS	THR	engineered mutation	UNP P16218
D	1	MET	-	initiating methionine	UNP P16218
D	2	GLY	-	expression tag	UNP P16218
D	3	SER	-	expression tag	UNP P16218
D	4	SER	-	expression tag	UNP P16218
D	5	HIS	-	expression tag	UNP P16218
D	6	HIS	-	expression tag	UNP P16218
D	7	HIS	-	expression tag	UNP P16218
D	8	HIS	-	expression tag	UNP P16218
D	9	HIS	-	expression tag	UNP P16218
D	10	HIS	-	expression tag	UNP P16218
D	11	SER	-	expression tag	UNP P16218
D	12	SER	-	expression tag	UNP P16218
D	13	GLY	-	expression tag	UNP P16218
D	14	LEU	-	expression tag	UNP P16218
D	15	VAL	-	expression tag	UNP P16218
D	16	PRO	-	expression tag	UNP P16218
D	17	ARG	-	expression tag	UNP P16218
D	18	GLY	-	expression tag	UNP P16218
D	19	SER	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P16218
D	21	MET	-	expression tag	UNP P16218
D	22	ALA	-	expression tag	UNP P16218
D	23	SER	-	expression tag	UNP P16218
D	24	MET	-	expression tag	UNP P16218
D	25	THR	-	expression tag	UNP P16218
D	26	GLY	-	expression tag	UNP P16218
D	27	GLY	-	expression tag	UNP P16218
D	28	GLN	-	expression tag	UNP P16218
D	29	GLN	-	expression tag	UNP P16218
D	30	MET	-	expression tag	UNP P16218
D	31	GLY	-	expression tag	UNP P16218
D	32	ARG	-	expression tag	UNP P16218
D	33	ILE	-	expression tag	UNP P16218
D	34	GLU	-	expression tag	UNP P16218
D	35	GLY	-	expression tag	UNP P16218
D	36	ARG	-	expression tag	UNP P16218
D	37	GLU	-	expression tag	UNP P16218
D	38	PHE	-	expression tag	UNP P16218
D	267	ALA	PHE	engineered mutation	UNP P16218
D	273	PHE	TYR	engineered mutation	UNP P16218
D	278	GLN	-	insertion	UNP P16218
D	279	GLY	-	insertion	UNP P16218
D	280	ALA	-	insertion	UNP P16218
D	281	GLU	-	insertion	UNP P16218
D	282	TRP	-	insertion	UNP P16218
D	283	VAL	-	insertion	UNP P16218
D	284	GLU	-	insertion	UNP P16218
D	285	GLY	-	insertion	UNP P16218
D	286	SER	-	insertion	UNP P16218
D	287	GLU	-	insertion	UNP P16218
D	288	LYS	-	insertion	UNP P16218
D	289	TRP	LYS	engineered mutation	UNP P16218
D	290	LEU	TRP	engineered mutation	UNP P16218
D	291	GLY	ARG	engineered mutation	UNP P16218
D	292	ARG	GLY	engineered mutation	UNP P16218
D	293	LYS	THR	engineered mutation	UNP P16218
E	1	MET	-	initiating methionine	UNP P16218
E	2	GLY	-	expression tag	UNP P16218
E	3	SER	-	expression tag	UNP P16218
E	4	SER	-	expression tag	UNP P16218
E	5	HIS	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	HIS	-	expression tag	UNP P16218
E	7	HIS	-	expression tag	UNP P16218
E	8	HIS	-	expression tag	UNP P16218
E	9	HIS	-	expression tag	UNP P16218
E	10	HIS	-	expression tag	UNP P16218
E	11	SER	-	expression tag	UNP P16218
E	12	SER	-	expression tag	UNP P16218
E	13	GLY	-	expression tag	UNP P16218
E	14	LEU	-	expression tag	UNP P16218
E	15	VAL	-	expression tag	UNP P16218
E	16	PRO	-	expression tag	UNP P16218
E	17	ARG	-	expression tag	UNP P16218
E	18	GLY	-	expression tag	UNP P16218
E	19	SER	-	expression tag	UNP P16218
E	20	HIS	-	expression tag	UNP P16218
E	21	MET	-	expression tag	UNP P16218
E	22	ALA	-	expression tag	UNP P16218
E	23	SER	-	expression tag	UNP P16218
E	24	MET	-	expression tag	UNP P16218
E	25	THR	-	expression tag	UNP P16218
E	26	GLY	-	expression tag	UNP P16218
E	27	GLY	-	expression tag	UNP P16218
E	28	GLN	-	expression tag	UNP P16218
E	29	GLN	-	expression tag	UNP P16218
E	30	MET	-	expression tag	UNP P16218
E	31	GLY	-	expression tag	UNP P16218
E	32	ARG	-	expression tag	UNP P16218
E	33	ILE	-	expression tag	UNP P16218
E	34	GLU	-	expression tag	UNP P16218
E	35	GLY	-	expression tag	UNP P16218
E	36	ARG	-	expression tag	UNP P16218
E	37	GLU	-	expression tag	UNP P16218
E	38	PHE	-	expression tag	UNP P16218
E	267	ALA	PHE	engineered mutation	UNP P16218
E	273	PHE	TYR	engineered mutation	UNP P16218
E	278	GLN	-	insertion	UNP P16218
E	279	GLY	-	insertion	UNP P16218
E	280	ALA	-	insertion	UNP P16218
E	281	GLU	-	insertion	UNP P16218
E	282	TRP	-	insertion	UNP P16218
E	283	VAL	-	insertion	UNP P16218
E	284	GLU	-	insertion	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
E	285	GLY	-	insertion	UNP P16218
E	286	SER	-	insertion	UNP P16218
E	287	GLU	-	insertion	UNP P16218
E	288	LYS	-	insertion	UNP P16218
E	289	TRP	LYS	engineered mutation	UNP P16218
E	290	LEU	TRP	engineered mutation	UNP P16218
E	291	GLY	ARG	engineered mutation	UNP P16218
E	292	ARG	GLY	engineered mutation	UNP P16218
E	293	LYS	THR	engineered mutation	UNP P16218

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	36	Total O 36 36	0	0
2	B	54	Total O 54 54	0	0
2	C	19	Total O 19 19	0	0
2	D	23	Total O 23 23	0	0
2	E	44	Total O 44 44	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	222.32Å 222.32Å 207.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.60) 99.7 (20.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.209 , 0.260 0.214 , 0.263	Depositor DCC
R_{free} test set	4551 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13396	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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	0.79	0/2714	0.98	3/3683 (0.1%)
1	B	0.83	0/2698	0.97	2/3661 (0.1%)
1	C	0.78	0/2709	1.01	3/3676 (0.1%)
1	D	0.81	0/2723	1.05	4/3694 (0.1%)
1	E	0.76	0/2754	1.00	2/3739 (0.1%)
All	All	0.80	0/13598	1.00	14/18453 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	375	ARG	CG-CD-NE	6.76	126.86	112.00
1	E	187	ILE	N-CA-C	-6.66	103.84	110.30
1	E	166	ASN	N-CA-C	6.11	116.30	108.24
1	B	225	ARG	N-CA-C	5.89	117.79	111.36
1	A	92	GLY	N-CA-C	5.75	118.65	112.33
1	B	187	ILE	CB-CA-C	-5.69	104.41	111.70
1	C	77	ASP	CA-C-N	5.32	125.38	119.32
1	C	77	ASP	C-N-CA	5.32	125.38	119.32
1	D	166	ASN	N-CA-C	5.28	114.81	107.73
1	D	390	ASN	CA-C-N	5.25	125.17	119.76
1	D	390	ASN	C-N-CA	5.25	125.17	119.76
1	A	378	ARG	CG-CD-NE	5.17	123.37	112.00
1	A	187	ILE	CB-CA-C	-5.13	105.13	111.70
1	C	166	ASN	N-CA-C	5.03	114.78	108.45

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	2639	0	2486	29	0
1	B	2623	0	2471	22	0
1	C	2634	0	2481	33	0
1	D	2648	0	2499	29	0
1	E	2676	0	2516	23	0
2	A	36	0	0	0	0
2	B	54	0	0	1	0
2	C	19	0	0	0	0
2	D	23	0	0	0	0
2	E	44	0	0	1	0
All	All	13396	0	12453	135	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 5.

All (135) 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:A:133:THR:HG21	1:A:187:ILE:CD1	2.17	0.74
1:D:113:ASP:OD1	1:D:159:ARG:NH2	2.23	0.71
1:B:133:THR:HG21	1:B:187:ILE:CD1	2.23	0.69
1:E:133:THR:HG21	1:E:187:ILE:CD1	2.26	0.66
1:D:133:THR:HG21	1:D:187:ILE:HD11	1.77	0.65
1:C:392:GLY:O	1:C:393:THR:HG23	1.95	0.65
1:A:308:ASP:OD1	1:A:351:ARG:NH1	2.31	0.62
1:C:243:GLY:C	1:C:251:THR:HG21	2.25	0.61
1:D:111:TYR:CZ	1:D:375:ARG:HD3	2.35	0.61
1:E:134:MET:SD	1:E:140:THR:HG23	2.41	0.61
1:B:169:HIS:HD2	2:B:515:HOH:O	1.83	0.61
1:C:122:ASN:ND2	1:C:356:SER:OG	2.28	0.60
1:B:231:ARG:NH2	1:B:237:ARG:O	2.35	0.60
1:B:133:THR:HG21	1:B:187:ILE:HD11	1.84	0.59
1:D:133:THR:HG21	1:D:187:ILE:CD1	2.33	0.58
1:A:243:GLY:HA3	1:A:251:THR:HG23	1.85	0.57
1:C:365:SER:HB2	1:C:367:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:TYR:O	1:D:345:SER:HB2	2.04	0.57
1:B:147:ASP:OD1	1:B:194:ARG:NH2	2.38	0.57
1:A:134:MET:CE	1:A:140:THR:HB	2.35	0.57
1:B:243:GLY:HA3	1:B:251:THR:HG23	1.86	0.56
1:C:269:TYR:CE1	1:C:271:ASP:HB2	2.39	0.56
1:A:243:GLY:C	1:A:251:THR:HG21	2.30	0.56
1:A:244:GLY:O	1:A:251:THR:HG21	2.05	0.56
1:B:244:GLY:N	1:B:251:THR:HG21	2.21	0.55
1:A:114:ASP:OD1	1:A:378:ARG:NH1	2.40	0.55
1:B:341:TYR:O	1:B:345:SER:OG	2.25	0.55
1:A:207:MET:HE2	1:A:210:PRO:HG3	1.88	0.54
1:A:244:GLY:N	1:A:251:THR:HG21	2.23	0.54
1:B:207:MET:HE2	1:B:210:PRO:HG3	1.89	0.54
1:B:109:GLU:HG2	1:B:159:ARG:HH22	1.73	0.54
1:A:76:VAL:HG21	1:A:200:GLU:HG3	1.89	0.54
1:A:133:THR:HG21	1:A:187:ILE:HD11	1.89	0.53
1:C:109:GLU:OE1	1:C:159:ARG:NH2	2.42	0.53
1:C:266:THR:HG22	1:C:322:TYR:O	2.09	0.53
1:D:243:GLY:HA3	1:D:251:THR:HG23	1.91	0.53
1:E:133:THR:HG21	1:E:187:ILE:HD11	1.90	0.53
1:B:130:ASP:OD1	1:B:183:ARG:NH2	2.39	0.53
1:E:221:ASP:O	1:E:225:ARG:HG3	2.09	0.52
1:B:135:ARG:HD3	2:E:502:HOH:O	2.10	0.51
1:B:243:GLY:C	1:B:251:THR:HG21	2.35	0.51
1:C:215:THR:HG22	1:C:218:GLN:H	1.75	0.51
1:C:280:ALA:HA	1:C:329:MET:HE2	1.92	0.51
1:C:244:GLY:O	1:C:251:THR:HG21	2.11	0.50
1:E:174:LYS:HD3	1:E:210:PRO:HA	1.94	0.50
1:D:96:GLU:OE2	1:D:358:TRP:HH2	1.95	0.50
1:B:346:ASP:OD2	1:B:391:PRO:HA	2.12	0.49
1:D:308:ASP:OD1	1:D:351:ARG:NH1	2.45	0.49
1:C:297:GLN:NE2	1:C:297:GLN:HA	2.26	0.49
1:D:221:ASP:O	1:D:225:ARG:HG3	2.13	0.49
1:E:166:ASN:OD1	1:E:166:ASN:C	2.55	0.49
1:C:274:GLU:HG2	1:C:289:TRP:CD2	2.48	0.49
1:C:114:ASP:OD2	1:C:373:TYR:OH	2.25	0.49
1:C:243:GLY:HA3	1:C:251:THR:HG23	1.95	0.49
1:A:134:MET:HE3	1:A:140:THR:HB	1.93	0.48
1:B:198:LYS:O	1:B:237:ARG:NH2	2.47	0.48
1:E:342:ASP:HB2	1:E:387:ALA:HB1	1.95	0.48
1:A:168:HIS:O	1:A:169:HIS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:OD2	1:A:378:ARG:HG3	2.13	0.48
1:D:139:TYR:CD1	1:D:183:ARG:HG3	2.48	0.48
1:E:209:GLU:OE2	1:E:268:HIS:HD2	1.97	0.48
1:A:80:GLU:O	1:A:83:ARG:HB2	2.14	0.48
1:E:307:PHE:CZ	1:E:323:PHE:HE2	2.32	0.48
1:C:114:ASP:OD2	1:C:378:ARG:HG3	2.14	0.48
1:C:130:ASP:OD1	1:C:183:ARG:NH2	2.46	0.48
1:D:167:SER:OG	1:D:170:ASP:OD2	2.32	0.48
1:E:207:MET:CE	1:E:210:PRO:HB3	2.44	0.48
1:C:82:VAL:HG21	1:C:320:PRO:HB2	1.96	0.47
1:C:249:TYR:CE2	1:C:306:VAL:HG13	2.50	0.47
1:A:134:MET:HE3	1:A:140:THR:CB	2.45	0.47
1:E:365:SER:HB2	1:E:367:ASP:HB2	1.96	0.47
1:B:243:GLY:HA3	1:B:251:THR:CG2	2.44	0.47
1:D:164:ILE:HD13	1:D:322:TYR:OH	2.15	0.47
1:C:243:GLY:C	1:C:251:THR:CG2	2.88	0.46
1:D:124:ARG:NH2	1:D:325:GLU:OE2	2.48	0.46
1:B:133:THR:O	1:E:135:ARG:NH2	2.39	0.46
1:D:145:PHE:O	1:D:149:VAL:HG23	2.14	0.46
1:D:166:ASN:C	1:D:166:ASN:OD1	2.59	0.46
1:C:196:LYS:HA	1:C:234:ASN:OD1	2.15	0.46
1:A:243:GLY:HA3	1:A:251:THR:CG2	2.44	0.45
1:D:109:GLU:OE1	1:D:159:ARG:NH1	2.49	0.45
1:A:134:MET:HE2	1:A:140:THR:HB	1.98	0.45
1:C:274:GLU:HG2	1:C:289:TRP:CE2	2.50	0.45
1:D:307:PHE:CZ	1:D:323:PHE:HE2	2.34	0.45
1:A:209:GLU:OE2	1:A:268:HIS:HD2	2.00	0.45
1:D:110:TYR:CE1	1:D:378:ARG:HD2	2.52	0.45
1:D:177:TYR:CZ	1:D:181:ILE:HD13	2.52	0.44
1:A:99:TYR:O	1:A:102:SER:OG	2.34	0.44
1:D:321:VAL:HB	1:D:353:PHE:CD1	2.52	0.44
1:B:244:GLY:O	1:B:251:THR:HG21	2.17	0.44
1:C:347:ALA:O	1:C:351:ARG:HG2	2.18	0.44
1:D:243:GLY:C	1:D:251:THR:HG21	2.42	0.44
1:C:271:ASP:HA	1:C:272:PRO:C	2.42	0.44
1:C:110:TYR:CD1	1:C:378:ARG:HD2	2.53	0.43
1:C:207:MET:HE2	1:C:210:PRO:HG3	1.99	0.43
1:D:244:GLY:O	1:D:251:THR:HG21	2.17	0.43
1:D:149:VAL:O	1:D:153:VAL:HG23	2.18	0.43
1:A:166:ASN:OD1	1:A:166:ASN:C	2.61	0.43
1:D:97:ALA:O	1:D:98:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLY:C	1:A:251:THR:CG2	2.92	0.43
1:C:223:ASN:ND2	1:C:241:ILE:HG22	2.34	0.42
1:C:305:ARG:HH11	1:C:305:ARG:HB2	1.83	0.42
1:C:85:MET:HG2	1:C:162:VAL:HG11	2.00	0.42
1:A:327:ALA:HB2	1:A:358:TRP:HB3	2.01	0.42
1:B:207:MET:HE2	1:B:210:PRO:CG	2.47	0.42
1:E:97:ALA:O	1:E:98:PRO:C	2.60	0.42
1:E:207:MET:CE	1:E:210:PRO:HG3	2.50	0.42
1:C:251:THR:HG22	1:C:252:LEU:N	2.35	0.42
1:A:269:TYR:CZ	1:A:271:ASP:HB2	2.54	0.42
1:A:134:MET:HE3	1:A:140:THR:H	1.84	0.42
1:B:207:MET:HE2	1:B:210:PRO:CB	2.50	0.42
1:C:305:ARG:HH11	1:C:305:ARG:CB	2.33	0.42
1:A:207:MET:HE2	1:A:210:PRO:HB3	2.02	0.41
1:A:283:VAL:O	1:A:286:SER:OG	2.38	0.41
1:C:110:TYR:CE1	1:C:378:ARG:HD2	2.55	0.41
1:E:159:ARG:HH11	1:E:159:ARG:HG3	1.84	0.41
1:B:116:LYS:HD2	1:B:159:ARG:HB3	2.02	0.41
1:D:314:SER:OG	1:D:319:ILE:O	2.32	0.41
1:E:207:MET:HE1	1:E:210:PRO:HB3	2.01	0.41
1:E:308:ASP:OD1	1:E:351:ARG:NH1	2.53	0.41
1:E:321:VAL:HB	1:E:353:PHE:CD1	2.55	0.41
1:B:234:ASN:OD1	1:B:237:ARG:NH1	2.51	0.41
1:E:319:ILE:HA	1:E:320:PRO:HD3	1.95	0.41
1:E:305:ARG:HH11	1:E:305:ARG:HG2	1.86	0.41
1:E:332:ALA:O	1:E:333:ASP:C	2.64	0.41
1:A:365:SER:HB2	1:A:367:ASP:HB2	2.03	0.41
1:D:332:ALA:O	1:D:333:ASP:C	2.63	0.41
1:E:207:MET:HE3	1:E:210:PRO:CB	2.51	0.41
1:C:118:ALA:HB1	1:C:385:LEU:HD21	2.03	0.40
1:C:291:GLY:O	1:C:292:ARG:C	2.65	0.40
1:D:207:MET:HE2	1:D:210:PRO:HG3	2.04	0.40
1:D:365:SER:HB2	1:D:367:ASP:HB2	2.03	0.40
1:E:76:VAL:HG23	1:E:200:GLU:HG3	2.03	0.40
1:A:174:LYS:HG2	1:A:207:MET:HE3	2.02	0.40
1:D:82:VAL:HG21	1:D:320:PRO:HB2	2.03	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	317/414 (77%)	300 (95%)	16 (5%)	1 (0%)	36	58
1	B	314/414 (76%)	302 (96%)	12 (4%)	0	100	100
1	C	316/414 (76%)	292 (92%)	23 (7%)	1 (0%)	36	58
1	D	318/414 (77%)	289 (91%)	28 (9%)	1 (0%)	36	58
1	E	321/414 (78%)	301 (94%)	18 (6%)	2 (1%)	21	42
All	All	1586/2070 (77%)	1484 (94%)	97 (6%)	5 (0%)	36	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ASP
1	C	367	ASP
1	D	367	ASP
1	E	86	GLY
1	E	367	ASP

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	281/361 (78%)	267 (95%)	14 (5%)	22	46
1	B	280/361 (78%)	264 (94%)	16 (6%)	18	40
1	C	281/361 (78%)	259 (92%)	22 (8%)	11	26
1	D	282/361 (78%)	265 (94%)	17 (6%)	17	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	285/361 (79%)	266 (93%)	19 (7%)	15	33
All	All	1409/1805 (78%)	1321 (94%)	88 (6%)	16	36

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	102	SER
1	A	135	ARG
1	A	225	ARG
1	A	251	THR
1	A	253	VAL
1	A	281	GLU
1	A	305	ARG
1	A	312	SER
1	A	344	ILE
1	A	351	ARG
1	A	365	SER
1	A	378	ARG
1	A	393	THR
1	B	82	VAL
1	B	83	ARG
1	B	183	ARG
1	B	199	SER
1	B	203	LEU
1	B	225	ARG
1	B	228	LYS
1	B	230	ILE
1	B	251	THR
1	B	281	GLU
1	B	292	ARG
1	B	333	ASP
1	B	337	ARG
1	B	339	LYS
1	B	345	SER
1	B	366	LEU
1	C	82	VAL
1	C	121	LYS
1	C	135	ARG
1	C	183	ARG
1	C	199	SER
1	C	215	THR

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Mol	Chain	Res	Type
1	C	225	ARG
1	C	236	THR
1	C	250	ASN
1	C	251	THR
1	C	253	VAL
1	C	289	TRP
1	C	293	LYS
1	C	297	GLN
1	C	298	GLU
1	C	300	MET
1	C	305	ARG
1	C	312	SER
1	C	319	ILE
1	C	331	TYR
1	C	335	THR
1	C	378	ARG
1	D	82	VAL
1	D	135	ARG
1	D	159	ARG
1	D	181	ILE
1	D	225	ARG
1	D	229	ILE
1	D	251	THR
1	D	298	GLU
1	D	305	ARG
1	D	311	LYS
1	D	345	SER
1	D	351	ARG
1	D	365	SER
1	D	375	ARG
1	D	378	ARG
1	D	382	THR
1	D	393	THR
1	E	82	VAL
1	E	94	THR
1	E	121	LYS
1	E	135	ARG
1	E	140	THR
1	E	159	ARG
1	E	187	ILE
1	E	225	ARG
1	E	232	LYS

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Mol	Chain	Res	Type
1	E	250	ASN
1	E	281	GLU
1	E	298	GLU
1	E	305	ARG
1	E	311	LYS
1	E	333	ASP
1	E	351	ARG
1	E	365	SER
1	E	378	ARG
1	E	396	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	278	GLN
1	A	297	GLN
1	A	368	ASN
1	B	132	HIS
1	B	169	HIS
1	B	250	ASN
1	B	317	ASN
1	B	368	ASN
1	B	390	ASN
1	C	197	ASN
1	C	213	ASN
1	C	223	ASN
1	C	297	GLN
1	C	368	ASN
1	D	151	GLN
1	D	180	ASN
1	D	208	ASN
1	D	213	ASN
1	D	368	ASN
1	D	390	ASN
1	E	151	GLN
1	E	213	ASN

5.3.3 RNA ⓘ

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	319/414 (77%)	-0.31	1 (0%) 90 88	31, 45, 61, 79	0
1	B	316/414 (76%)	-0.52	0 100 100	30, 38, 54, 70	0
1	C	318/414 (76%)	0.22	6 (1%) 66 61	36, 55, 74, 89	0
1	D	320/414 (77%)	0.30	3 (0%) 81 78	35, 55, 76, 93	0
1	E	323/414 (78%)	-0.12	2 (0%) 85 83	33, 48, 68, 105	0
All	All	1596/2070 (77%)	-0.09	12 (0%) 82 80	30, 48, 71, 105	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	397	TYR	4.9
1	C	76	VAL	3.5
1	C	393	THR	3.2
1	D	393	THR	2.9
1	C	343	PHE	2.7
1	C	298	GLU	2.5
1	A	393	THR	2.5
1	D	262	TYR	2.4
1	D	74	LYS	2.3
1	C	297	GLN	2.2
1	C	387	ALA	2.2
1	E	396	SER	2.1

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.