



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:35 PM UTC

PDB ID : 3DED / pdb_00003ded
Title : C-terminal domain of Probable hemolysin from *Chromobacterium violaceum*
Authors : Chang, C.; Xu, X.; Cui, H.; Savchenko, A.; Edwards, A.; Joachimiak, A.;
Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-06-09
Resolution : 2.14 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
Mogul : 2022.3.0, CSD as543be (2022)
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

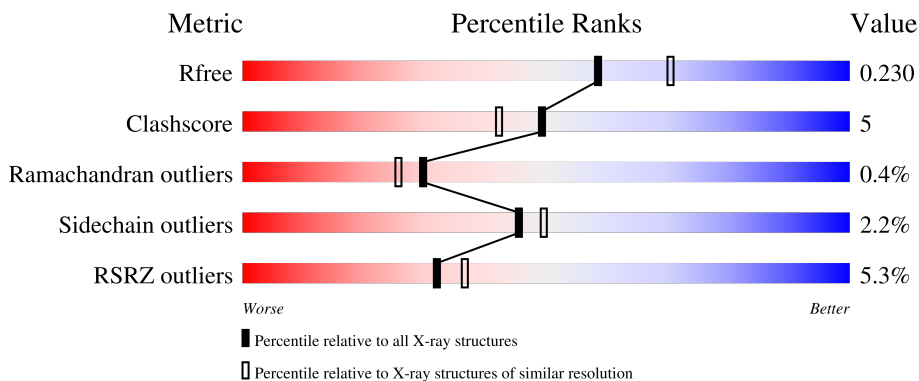
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

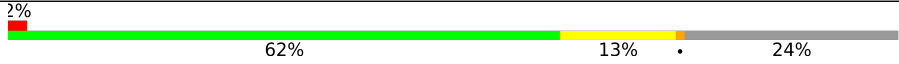
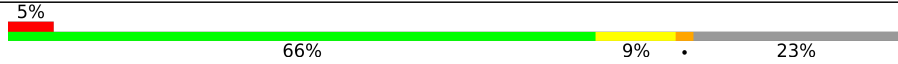
The reported resolution of this entry is 2.14 Å.

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.



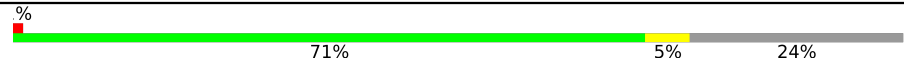
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	113	
1	B	113	
1	C	113	
1	D	113	
1	E	113	

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Mol	Chain	Length	Quality of chain
1	F	113	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '71%', a yellow segment in the middle labeled '5%', and a grey segment on the right labeled '24%'. A small red square is at the beginning of the bar, and a '%' symbol is above it.</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4716 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 Probable hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	87	Total 713	C 450	N 125	O 135	Se 3	0	2	0
1	B	86	Total 707	C 449	N 122	O 133	Se 3	0	3	0
1	C	91	Total 725	C 455	N 127	O 140	Se 3	0	0	0
1	D	86	Total 687	C 434	N 119	O 131	Se 3	0	0	0
1	E	87	Total 716	C 452	N 128	O 133	Se 3	0	2	0
1	F	86	Total 707	C 446	N 123	O 134	Se 4	0	2	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	MSE	-	expression tag	UNP Q7P1I2
A	316	GLY	-	expression tag	UNP Q7P1I2
A	317	SER	-	expression tag	UNP Q7P1I2
A	318	SER	-	expression tag	UNP Q7P1I2
A	319	HIS	-	expression tag	UNP Q7P1I2
A	320	HIS	-	expression tag	UNP Q7P1I2
A	321	HIS	-	expression tag	UNP Q7P1I2
A	322	HIS	-	expression tag	UNP Q7P1I2
A	323	HIS	-	expression tag	UNP Q7P1I2
A	324	HIS	-	expression tag	UNP Q7P1I2
A	325	SER	-	expression tag	UNP Q7P1I2
A	326	SER	-	expression tag	UNP Q7P1I2
A	327	GLY	-	expression tag	UNP Q7P1I2
A	328	ARG	-	expression tag	UNP Q7P1I2
A	329	GLU	-	expression tag	UNP Q7P1I2
A	330	ASN	-	expression tag	UNP Q7P1I2
A	331	LEU	-	expression tag	UNP Q7P1I2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	332	TYR	-	expression tag	UNP Q7P1I2
A	333	PHE	-	expression tag	UNP Q7P1I2
A	334	GLN	-	expression tag	UNP Q7P1I2
A	335	GLY	-	expression tag	UNP Q7P1I2
A	336	HIS	-	expression tag	UNP Q7P1I2
B	315	MSE	-	expression tag	UNP Q7P1I2
B	316	GLY	-	expression tag	UNP Q7P1I2
B	317	SER	-	expression tag	UNP Q7P1I2
B	318	SER	-	expression tag	UNP Q7P1I2
B	319	HIS	-	expression tag	UNP Q7P1I2
B	320	HIS	-	expression tag	UNP Q7P1I2
B	321	HIS	-	expression tag	UNP Q7P1I2
B	322	HIS	-	expression tag	UNP Q7P1I2
B	323	HIS	-	expression tag	UNP Q7P1I2
B	324	HIS	-	expression tag	UNP Q7P1I2
B	325	SER	-	expression tag	UNP Q7P1I2
B	326	SER	-	expression tag	UNP Q7P1I2
B	327	GLY	-	expression tag	UNP Q7P1I2
B	328	ARG	-	expression tag	UNP Q7P1I2
B	329	GLU	-	expression tag	UNP Q7P1I2
B	330	ASN	-	expression tag	UNP Q7P1I2
B	331	LEU	-	expression tag	UNP Q7P1I2
B	332	TYR	-	expression tag	UNP Q7P1I2
B	333	PHE	-	expression tag	UNP Q7P1I2
B	334	GLN	-	expression tag	UNP Q7P1I2
B	335	GLY	-	expression tag	UNP Q7P1I2
B	336	HIS	-	expression tag	UNP Q7P1I2
C	315	MSE	-	expression tag	UNP Q7P1I2
C	316	GLY	-	expression tag	UNP Q7P1I2
C	317	SER	-	expression tag	UNP Q7P1I2
C	318	SER	-	expression tag	UNP Q7P1I2
C	319	HIS	-	expression tag	UNP Q7P1I2
C	320	HIS	-	expression tag	UNP Q7P1I2
C	321	HIS	-	expression tag	UNP Q7P1I2
C	322	HIS	-	expression tag	UNP Q7P1I2
C	323	HIS	-	expression tag	UNP Q7P1I2
C	324	HIS	-	expression tag	UNP Q7P1I2
C	325	SER	-	expression tag	UNP Q7P1I2
C	326	SER	-	expression tag	UNP Q7P1I2
C	327	GLY	-	expression tag	UNP Q7P1I2
C	328	ARG	-	expression tag	UNP Q7P1I2
C	329	GLU	-	expression tag	UNP Q7P1I2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	330	ASN	-	expression tag	UNP Q7P1I2
C	331	LEU	-	expression tag	UNP Q7P1I2
C	332	TYR	-	expression tag	UNP Q7P1I2
C	333	PHE	-	expression tag	UNP Q7P1I2
C	334	GLN	-	expression tag	UNP Q7P1I2
C	335	GLY	-	expression tag	UNP Q7P1I2
C	336	HIS	-	expression tag	UNP Q7P1I2
D	315	MSE	-	expression tag	UNP Q7P1I2
D	316	GLY	-	expression tag	UNP Q7P1I2
D	317	SER	-	expression tag	UNP Q7P1I2
D	318	SER	-	expression tag	UNP Q7P1I2
D	319	HIS	-	expression tag	UNP Q7P1I2
D	320	HIS	-	expression tag	UNP Q7P1I2
D	321	HIS	-	expression tag	UNP Q7P1I2
D	322	HIS	-	expression tag	UNP Q7P1I2
D	323	HIS	-	expression tag	UNP Q7P1I2
D	324	HIS	-	expression tag	UNP Q7P1I2
D	325	SER	-	expression tag	UNP Q7P1I2
D	326	SER	-	expression tag	UNP Q7P1I2
D	327	GLY	-	expression tag	UNP Q7P1I2
D	328	ARG	-	expression tag	UNP Q7P1I2
D	329	GLU	-	expression tag	UNP Q7P1I2
D	330	ASN	-	expression tag	UNP Q7P1I2
D	331	LEU	-	expression tag	UNP Q7P1I2
D	332	TYR	-	expression tag	UNP Q7P1I2
D	333	PHE	-	expression tag	UNP Q7P1I2
D	334	GLN	-	expression tag	UNP Q7P1I2
D	335	GLY	-	expression tag	UNP Q7P1I2
D	336	HIS	-	expression tag	UNP Q7P1I2
E	315	MSE	-	expression tag	UNP Q7P1I2
E	316	GLY	-	expression tag	UNP Q7P1I2
E	317	SER	-	expression tag	UNP Q7P1I2
E	318	SER	-	expression tag	UNP Q7P1I2
E	319	HIS	-	expression tag	UNP Q7P1I2
E	320	HIS	-	expression tag	UNP Q7P1I2
E	321	HIS	-	expression tag	UNP Q7P1I2
E	322	HIS	-	expression tag	UNP Q7P1I2
E	323	HIS	-	expression tag	UNP Q7P1I2
E	324	HIS	-	expression tag	UNP Q7P1I2
E	325	SER	-	expression tag	UNP Q7P1I2
E	326	SER	-	expression tag	UNP Q7P1I2
E	327	GLY	-	expression tag	UNP Q7P1I2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	328	ARG	-	expression tag	UNP Q7P1I2
E	329	GLU	-	expression tag	UNP Q7P1I2
E	330	ASN	-	expression tag	UNP Q7P1I2
E	331	LEU	-	expression tag	UNP Q7P1I2
E	332	TYR	-	expression tag	UNP Q7P1I2
E	333	PHE	-	expression tag	UNP Q7P1I2
E	334	GLN	-	expression tag	UNP Q7P1I2
E	335	GLY	-	expression tag	UNP Q7P1I2
E	336	HIS	-	expression tag	UNP Q7P1I2
F	315	MSE	-	expression tag	UNP Q7P1I2
F	316	GLY	-	expression tag	UNP Q7P1I2
F	317	SER	-	expression tag	UNP Q7P1I2
F	318	SER	-	expression tag	UNP Q7P1I2
F	319	HIS	-	expression tag	UNP Q7P1I2
F	320	HIS	-	expression tag	UNP Q7P1I2
F	321	HIS	-	expression tag	UNP Q7P1I2
F	322	HIS	-	expression tag	UNP Q7P1I2
F	323	HIS	-	expression tag	UNP Q7P1I2
F	324	HIS	-	expression tag	UNP Q7P1I2
F	325	SER	-	expression tag	UNP Q7P1I2
F	326	SER	-	expression tag	UNP Q7P1I2
F	327	GLY	-	expression tag	UNP Q7P1I2
F	328	ARG	-	expression tag	UNP Q7P1I2
F	329	GLU	-	expression tag	UNP Q7P1I2
F	330	ASN	-	expression tag	UNP Q7P1I2
F	331	LEU	-	expression tag	UNP Q7P1I2
F	332	TYR	-	expression tag	UNP Q7P1I2
F	333	PHE	-	expression tag	UNP Q7P1I2
F	334	GLN	-	expression tag	UNP Q7P1I2
F	335	GLY	-	expression tag	UNP Q7P1I2
F	336	HIS	-	expression tag	UNP Q7P1I2

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

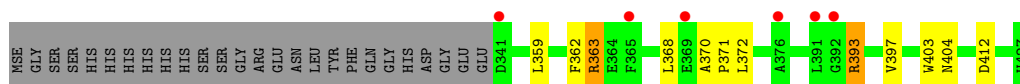
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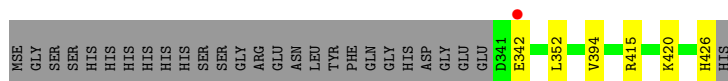
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Ca 2	0	0
2	F	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total 86	O 86	0	0
3	B	74	Total 74	O 74	0	0
3	C	54	Total 54	O 54	0	0
3	D	66	Total 66	O 66	0	0
3	E	85	Total 85	O 85	0	0
3	F	87	Total 87	O 87	0	0



- Molecule 1: Probable hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.14Å 55.31Å 93.73Å 90.00° 94.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.14 50.00 – 2.14	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.14) 98.2 (50.00-2.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.235 0.182 , 0.230	Depositor DCC
R_{free} test set	1847 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4716	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.86	1/732 (0.1%)	0.85	0/983
1	B	0.84	0/728	0.89	1/979 (0.1%)
1	C	0.78	0/737	0.91	0/990
1	D	0.79	0/699	0.97	0/940
1	E	0.84	0/735	0.93	0/986
1	F	0.86	0/722	0.90	0/969
All	All	0.83	1/4353 (0.0%)	0.91	1/5847 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	ALA	CA-CB	5.07	1.61	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ILE	N-CA-C	5.13	115.76	108.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	713	0	678	3	0
1	B	707	0	682	11	0
1	C	725	0	677	9	0
1	D	687	0	647	7	0
1	E	716	0	687	13	0
1	F	707	0	672	4	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	86	0	0	1	0
3	B	74	0	0	1	0
3	C	54	0	0	1	0
3	D	66	0	0	1	0
3	E	85	0	0	2	0
3	F	87	0	0	1	0
All	All	4716	0	4043	45	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 (45) 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:C:338:GLY:HA3	1:C:339:GLU:HB2	1.26	1.16
1:B:342[B]:GLU:HB2	1:B:357[B]:VAL:HG22	1.32	1.11
1:B:342[B]:GLU:HB2	1:B:357[B]:VAL:CG2	1.91	0.98
1:C:338:GLY:HA3	1:C:339:GLU:CB	1.97	0.87
1:C:338:GLY:CA	1:C:339:GLU:HB2	2.12	0.74
1:E:368:LEU:CD1	1:E:372:LEU:HD11	2.24	0.68
1:C:338:GLY:CA	1:C:339:GLU:CB	2.71	0.68
1:B:342[B]:GLU:OE2	3:B:517:HOH:O	2.12	0.67
1:E:362:PHE:HE2	1:E:368:LEU:HD11	1.61	0.65
1:E:368:LEU:HD13	1:E:372:LEU:HD11	1.79	0.65
1:A:342:GLU:HG2	1:A:354[B]:ASP:OD2	1.97	0.63
1:D:363:ARG:HD3	1:D:370:ALA:O	2.01	0.60
1:E:404:ASN:HB2	3:E:568:HOH:O	2.01	0.59
1:E:359:LEU:O	1:E:363:ARG:HB3	2.03	0.58
1:E:397[A]:VAL:CG1	1:F:352:LEU:HD13	2.35	0.56
1:B:386:VAL:HG12	1:B:387:MSE:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:GLU:HG2	1:C:361:ARG:HH22	1.72	0.54
1:B:400:ARG:HG3	1:B:409:GLU:HB2	1.88	0.54
1:E:362:PHE:CE2	1:E:368:LEU:HD11	2.43	0.54
1:B:394:VAL:O	1:B:394:VAL:HG13	2.07	0.54
1:B:342[B]:GLU:CB	1:B:357[B]:VAL:HG22	2.22	0.53
1:F:415:ARG:HH11	1:F:415:ARG:HG3	1.74	0.52
1:D:400:ARG:NH1	3:D:574:HOH:O	2.43	0.52
1:E:363:ARG:HH22	1:E:370:ALA:C	2.17	0.51
1:C:354:ASP:OD1	3:C:537:HOH:O	2.18	0.51
1:D:363:ARG:NH2	1:D:375:GLU:OE2	2.44	0.51
1:D:394:VAL:HG13	1:D:394:VAL:O	2.11	0.51
1:E:404:ASN:CB	3:E:568:HOH:O	2.59	0.50
1:E:359:LEU:HD22	1:E:372:LEU:HD22	1.95	0.49
1:C:363:ARG:NH2	1:C:375:GLU:OE2	2.43	0.47
1:E:371:PRO:O	1:E:403:TRP:CZ2	2.68	0.46
1:A:354[A]:ASP:OD2	3:A:526:HOH:O	2.20	0.46
1:D:363:ARG:HH21	1:D:375:GLU:CD	2.24	0.44
1:D:418:VAL:HG12	1:D:421:ILE:HD11	2.01	0.43
1:F:426:HIS:HD2	3:F:587:HOH:O	2.01	0.43
1:E:393[B]:ARG:HA	1:E:393[B]:ARG:HD2	1.73	0.43
1:B:400:ARG:NH2	1:B:402:GLU:OE2	2.52	0.42
1:B:363:ARG:HD3	1:B:370:ALA:O	2.19	0.41
1:E:412:ASP:OD1	1:F:420:LYS:HE2	2.20	0.41
1:A:363:ARG:NH2	1:A:375:GLU:OE2	2.54	0.41
1:C:393:ARG:HA	1:C:393:ARG:HD2	1.81	0.41
1:C:400:ARG:HA	1:C:408:PHE:O	2.21	0.40
1:B:390:GLN:HG2	1:B:401:PHE:CD1	2.57	0.40
1:D:368:LEU:HD21	1:D:406:PHE:HE2	1.87	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	87/113 (77%)	84 (97%)	3 (3%)	0	100	100
1	B	87/113 (77%)	83 (95%)	4 (5%)	0	100	100
1	C	89/113 (79%)	81 (91%)	7 (8%)	1 (1%)	11	6
1	D	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
1	E	87/113 (77%)	84 (97%)	3 (3%)	0	100	100
1	F	86/113 (76%)	83 (96%)	2 (2%)	1 (1%)	10	5
All	All	520/678 (77%)	497 (96%)	21 (4%)	2 (0%)	30	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	339	GLU
1	F	342	GLU

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	77/94 (82%)	77 (100%)	0	100	100
1	B	77/94 (82%)	73 (95%)	4 (5%)	21	16
1	C	76/94 (81%)	74 (97%)	2 (3%)	40	42
1	D	73/94 (78%)	72 (99%)	1 (1%)	59	65
1	E	77/94 (82%)	74 (96%)	3 (4%)	28	26
1	F	76/94 (81%)	75 (99%)	1 (1%)	61	67
All	All	456/564 (81%)	445 (98%)	11 (2%)	45	45

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	361	ARG
1	B	400	ARG
1	B	424	GLN

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Mol	Chain	Res	Type
1	B	426	HIS
1	C	380	ILE
1	C	394	VAL
1	D	369	GLU
1	E	363	ARG
1	E	393[A]	ARG
1	E	393[B]	ARG
1	F	394	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	C	381	HIS
1	D	381	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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.

No monomer is involved in short contacts.

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	84/113 (74%)	0.01	0 100 100	13, 29, 37, 41	2 (2%)
1	B	83/113 (73%)	0.41	2 (2%) 59 63	14, 26, 38, 43	3 (3%)
1	C	88/113 (77%)	0.77	7 (7%) 18 21	26, 33, 49, 55	0
1	D	83/113 (73%)	0.69	11 (13%) 7 8	26, 31, 40, 47	0
1	E	84/113 (74%)	0.40	6 (7%) 22 25	16, 28, 39, 49	2 (2%)
1	F	83/113 (73%)	0.06	1 (1%) 76 80	15, 25, 38, 43	1 (1%)
All	All	505/678 (74%)	0.39	27 (5%) 32 36	13, 29, 41, 55	8 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	GLY	3.9
1	C	337	ASP	3.7
1	C	339	GLU	3.6
1	D	341	ASP	3.4
1	D	361	ARG	3.3
1	E	365	PHE	3.1
1	C	391	LEU	3.0
1	E	341	ASP	2.9
1	E	369	GLU	2.8
1	C	427	HIS	2.7
1	D	384	ALA	2.6
1	C	426	HIS	2.6
1	D	380	ILE	2.5
1	E	392	GLY	2.5
1	E	391	LEU	2.5
1	D	392	GLY	2.4
1	D	386	VAL	2.3
1	D	388	LEU	2.3
1	E	376	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	342[A]	GLU	2.2
1	D	342	GLU	2.1
1	D	357	VAL	2.1
1	D	391	LEU	2.1
1	C	378	GLY	2.1
1	D	383	LEU	2.0
1	F	342	GLU	2.0
1	B	378	GLY	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](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	505	1/1	0.98	0.08	20,20,20,20	0
2	CA	C	507	1/1	0.98	0.12	23,23,23,23	0
2	CA	F	503	1/1	0.98	0.08	24,24,24,24	0
2	CA	A	504	1/1	0.99	0.07	20,20,20,20	0
2	CA	C	508	1/1	0.99	0.06	26,26,26,26	0
2	CA	D	509	1/1	0.99	0.08	28,28,28,28	0
2	CA	E	501	1/1	0.99	0.08	24,24,24,24	0
2	CA	E	502	1/1	0.99	0.09	21,21,21,21	0
2	CA	B	506	1/1	0.99	0.06	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.