



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:07 AM GMT

PDB ID : 3DED  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

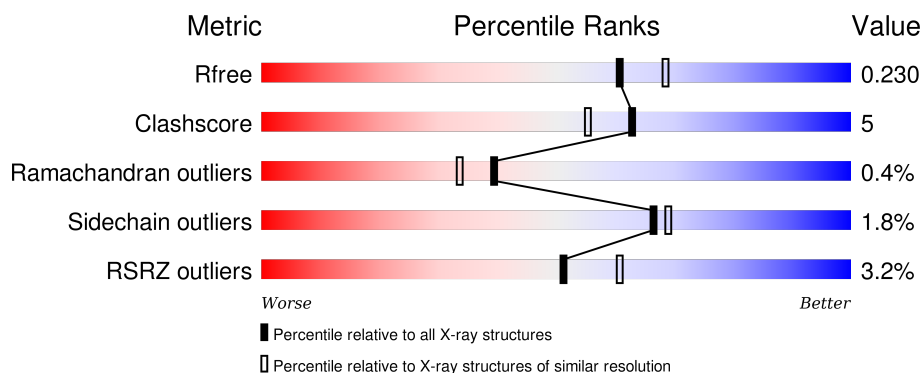
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>73%</div> <div>23%</div> </div>
1	B	113	<div> <div>3%</div> <div>63%</div> <div>12%</div> <div>24%</div> </div>
1	C	113	<div> <div>5%</div> <div>72%</div> <div>8%</div> <div>19%</div> </div>
1	D	113	<div> <div>68%</div> <div>8%</div> <div>24%</div> </div>
1	E	113	<div> <div>4%</div> <div>66%</div> <div>9%</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	113	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment representing 71%, a yellow segment representing 5%, and a grey segment representing 24%. The percentages are labeled below the bar.

## 2 Entry composition

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

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 (three-letter code: CA) (formula: Ca).

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

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

- Molecule 3 is water.

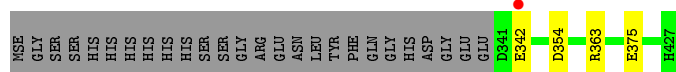
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total 86	O 86	0	0
3	B	74	Total 74	O 74	0	0
3	C	54	Total 54	O 54	0	0
3	D	66	Total 66	O 66	0	0
3	E	85	Total 85	O 85	0	0
3	F	87	Total 87	O 87	0	0



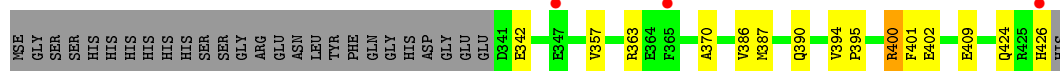
### 3 Residue-property plots [i](#)

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.

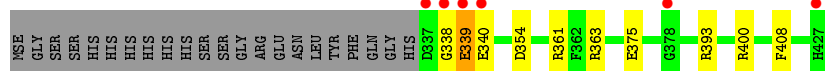
- Molecule 1: Probable hemolysin



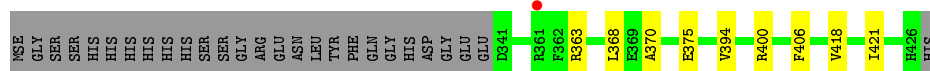
- Molecule 1: Probable hemolysin



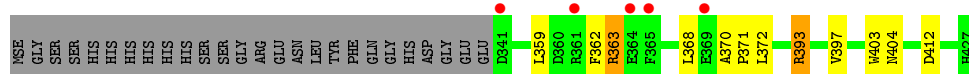
- Molecule 1: Probable hemolysin



- Molecule 1: Probable hemolysin



- Molecule 1: Probable hemolysin



- Molecule 1: Probable hemolysin

Chain F: 

71%

5%

24%

MSE	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	ARG	GLU	ASN	LEU	TYR	PHE	GLN	GLY	HIS	ASP	GLY	GLU	GLU	D341	E342	L352	V394	R415	K420	H426	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.14Å 55.31Å 93.73Å 90.00° 94.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.14 30.66 – 2.14	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.14) 97.9 (30.66-2.14)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.14Å)	Xtriage
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 (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36956 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.72	0/732	0.70	0/983
1	B	0.70	0/728	0.70	0/979
1	C	0.64	0/737	0.71	0/990
1	D	0.64	0/699	0.72	0/940
1	E	0.77	0/735	0.73	0/986
1	F	0.75	0/722	0.70	0/969
All	All	0.70	0/4353	0.71	0/5847

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 [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	6	0
1	E	716	0	687	13	0
1	F	707	0	672	4	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	44	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 (44) 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:394:VAL:HG13	1:B:394:VAL:O	2.07	0.55
1:C:339:GLU:HG2	1:C:361:ARG:HH22	1.72	0.54
1:B:386:VAL:HG12	1:B:387:MSE:HE2	1.88	0.54
1:E:362:PHE:CE2	1:E:368:LEU:HD11	2.43	0.54
1:B:400:ARG:HG3	1:B:409:GLU:HB2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:ARG:NH1	3:D:574:HOH:O	2.43	0.52
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:E:363:ARG:HH22	1:E:370:ALA:C	2.17	0.47
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: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:HD2	1:E:393[B]:ARG:HA	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%)	17	9
1	D	84/113 (74%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	87/113 (77%)	84 (97%)	3 (3%)	0	100	100
1	F	86/113 (76%)	83 (96%)	2 (2%)	1 (1%)	16	8
All	All	520/678 (77%)	497 (96%)	21 (4%)	2 (0%)	39	33

All (2) Ramachandran outliers are listed below:

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

### 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	77/94 (82%)	77 (100%)	0	100	100
1	B	77/94 (82%)	73 (95%)	4 (5%)	29	23
1	C	76/94 (81%)	75 (99%)	1 (1%)	76	80
1	D	73/94 (78%)	73 (100%)	0	100	100
1	E	77/94 (82%)	74 (96%)	3 (4%)	39	36
1	F	76/94 (81%)	75 (99%)	1 (1%)	76	80
All	All	456/564 (81%)	447 (98%)	9 (2%)	66	66

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	395	PRO
1	B	400	ARG
1	B	424	GLN
1	B	426	HIS
1	C	340	GLU
1	E	363	ARG
1	E	393[A]	ARG
1	E	393[B]	ARG

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Mol	Chain	Res	Type
1	F	394	VAL

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

### 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 carbohydrates 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	84/113 (74%)	0.01	1 (1%) 81 85	22, 29, 37, 41	0
1	B	83/113 (73%)	0.25	3 (3%) 46 56	21, 27, 38, 43	0
1	C	88/113 (77%)	0.48	6 (6%) 20 27	26, 33, 49, 55	0
1	D	83/113 (73%)	0.10	1 (1%) 81 85	26, 31, 40, 47	0
1	E	84/113 (74%)	0.37	5 (5%) 25 33	22, 28, 39, 49	0
1	F	83/113 (73%)	0.05	0 100 100	19, 25, 38, 43	0
All	All	505/678 (74%)	0.21	16 (3%) 51 61	19, 29, 41, 55	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	GLY	4.7
1	C	339	GLU	3.8
1	C	337	ASP	3.5
1	C	378	GLY	3.1
1	E	364	GLU	2.9
1	E	365	PHE	2.8
1	C	427	HIS	2.8
1	E	369	GLU	2.5
1	B	426	HIS	2.5
1	E	361	ARG	2.4
1	A	342	GLU	2.4
1	D	361	ARG	2.3
1	B	347	GLU	2.3
1	E	341	ASP	2.1
1	C	340	GLU	2.1
1	B	365	PHE	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	C	507	1/1	0.99	0.05	-2.21	23,23,23,23	0
2	CA	F	503	1/1	0.99	0.02	-2.57	24,24,24,24	0
2	CA	E	501	1/1	0.99	0.03	-2.68	24,24,24,24	0
2	CA	C	508	1/1	0.99	0.03	-2.97	26,26,26,26	0
2	CA	B	506	1/1	1.00	0.02	-3.01	22,22,22,22	0
2	CA	E	502	1/1	0.99	0.02	-3.06	21,21,21,21	0
2	CA	A	504	1/1	1.00	0.03	-3.66	20,20,20,20	0
2	CA	D	509	1/1	0.99	0.03	-4.34	28,28,28,28	0
2	CA	A	505	1/1	0.99	0.03	-4.93	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.