



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:55 PM GMT

PDB ID : 3VFF  
Title : BlaC E166A CDC-OMe Acyl-Intermediate Complex  
Authors : Mire, J.A.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2012-01-09  
Resolution : 2.78 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

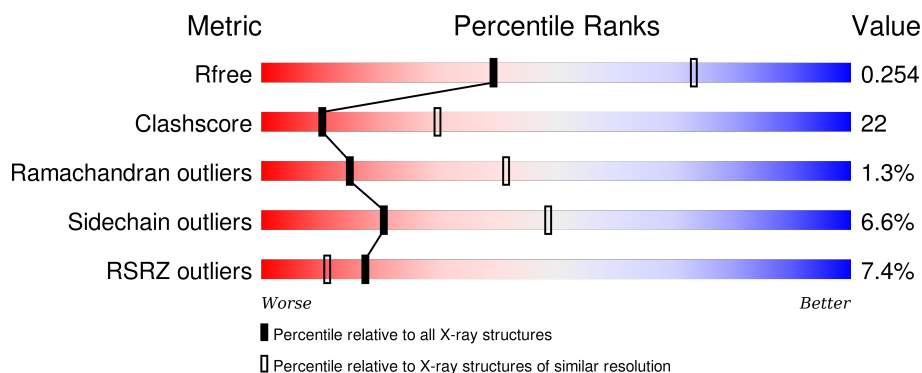
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	285	<div> <div>9%</div> <div>71%</div> <div>19%</div> <div>•</div> <div>7%</div> </div>
1	B	285	<div> <div>4%</div> <div>71%</div> <div>18%</div> <div>•</div> <div>10%</div> </div>
1	C	285	<div> <div>4%</div> <div>68%</div> <div>18%</div> <div>•</div> <div>10%</div> </div>
1	D	285	<div> <div>9%</div> <div>61%</div> <div>30%</div> <div>•</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CD8	A	301	-	-	X	-
2	CD8	B	301	-	-	X	X
2	CD8	C	301	-	-	X	X
2	CD8	D	301	-	-	X	-
3	PO4	B	302	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7409 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			1856	1167	331	352	6			
1	B	256	Total	C	N	O	S	0	0	0
			1793	1130	322	335	6			
1	C	256	Total	C	N	O	S	0	0	0
			1795	1137	317	335	6			
1	D	265	Total	C	N	O	S	0	0	0
			1841	1159	326	350	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	EXPRESSION TAG	UNP P0C5C1
A	10	GLY	-	EXPRESSION TAG	UNP P0C5C1
A	11	SER	-	EXPRESSION TAG	UNP P0C5C1
A	12	SER	-	EXPRESSION TAG	UNP P0C5C1
A	13	HIS	-	EXPRESSION TAG	UNP P0C5C1
A	14	HIS	-	EXPRESSION TAG	UNP P0C5C1
A	15	HIS	-	EXPRESSION TAG	UNP P0C5C1
A	16	HIS	-	EXPRESSION TAG	UNP P0C5C1
A	17	HIS	-	EXPRESSION TAG	UNP P0C5C1
A	18	HIS	-	EXPRESSION TAG	UNP P0C5C1
A	19	SER	-	EXPRESSION TAG	UNP P0C5C1
A	20	SER	-	EXPRESSION TAG	UNP P0C5C1
A	21	GLY	-	EXPRESSION TAG	UNP P0C5C1
A	22	GLU	-	EXPRESSION TAG	UNP P0C5C1
A	23	ASN	-	EXPRESSION TAG	UNP P0C5C1
A	24	LEU	-	EXPRESSION TAG	UNP P0C5C1
A	25	TYR	-	EXPRESSION TAG	UNP P0C5C1
A	26	PHE	-	EXPRESSION TAG	UNP P0C5C1
A	27	GLN	-	EXPRESSION TAG	UNP P0C5C1
A	28	GLY	-	EXPRESSION TAG	UNP P0C5C1
A	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1

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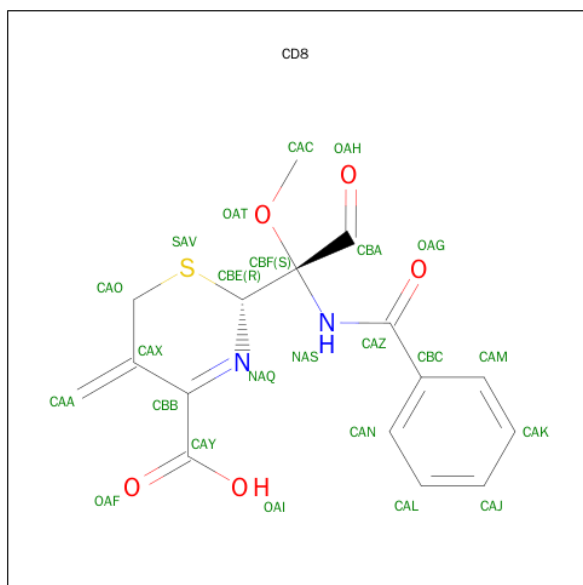
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	EXPRESSION TAG	UNP P0C5C1
B	10	GLY	-	EXPRESSION TAG	UNP P0C5C1
B	11	SER	-	EXPRESSION TAG	UNP P0C5C1
B	12	SER	-	EXPRESSION TAG	UNP P0C5C1
B	13	HIS	-	EXPRESSION TAG	UNP P0C5C1
B	14	HIS	-	EXPRESSION TAG	UNP P0C5C1
B	15	HIS	-	EXPRESSION TAG	UNP P0C5C1
B	16	HIS	-	EXPRESSION TAG	UNP P0C5C1
B	17	HIS	-	EXPRESSION TAG	UNP P0C5C1
B	18	HIS	-	EXPRESSION TAG	UNP P0C5C1
B	19	SER	-	EXPRESSION TAG	UNP P0C5C1
B	20	SER	-	EXPRESSION TAG	UNP P0C5C1
B	21	GLY	-	EXPRESSION TAG	UNP P0C5C1
B	22	GLU	-	EXPRESSION TAG	UNP P0C5C1
B	23	ASN	-	EXPRESSION TAG	UNP P0C5C1
B	24	LEU	-	EXPRESSION TAG	UNP P0C5C1
B	25	TYR	-	EXPRESSION TAG	UNP P0C5C1
B	26	PHE	-	EXPRESSION TAG	UNP P0C5C1
B	27	GLN	-	EXPRESSION TAG	UNP P0C5C1
B	28	GLY	-	EXPRESSION TAG	UNP P0C5C1
B	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1
C	9	MET	-	EXPRESSION TAG	UNP P0C5C1
C	10	GLY	-	EXPRESSION TAG	UNP P0C5C1
C	11	SER	-	EXPRESSION TAG	UNP P0C5C1
C	12	SER	-	EXPRESSION TAG	UNP P0C5C1
C	13	HIS	-	EXPRESSION TAG	UNP P0C5C1
C	14	HIS	-	EXPRESSION TAG	UNP P0C5C1
C	15	HIS	-	EXPRESSION TAG	UNP P0C5C1
C	16	HIS	-	EXPRESSION TAG	UNP P0C5C1
C	17	HIS	-	EXPRESSION TAG	UNP P0C5C1
C	18	HIS	-	EXPRESSION TAG	UNP P0C5C1
C	19	SER	-	EXPRESSION TAG	UNP P0C5C1
C	20	SER	-	EXPRESSION TAG	UNP P0C5C1
C	21	GLY	-	EXPRESSION TAG	UNP P0C5C1
C	22	GLU	-	EXPRESSION TAG	UNP P0C5C1
C	23	ASN	-	EXPRESSION TAG	UNP P0C5C1
C	24	LEU	-	EXPRESSION TAG	UNP P0C5C1
C	25	TYR	-	EXPRESSION TAG	UNP P0C5C1
C	26	PHE	-	EXPRESSION TAG	UNP P0C5C1
C	27	GLN	-	EXPRESSION TAG	UNP P0C5C1
C	28	GLY	-	EXPRESSION TAG	UNP P0C5C1
C	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1

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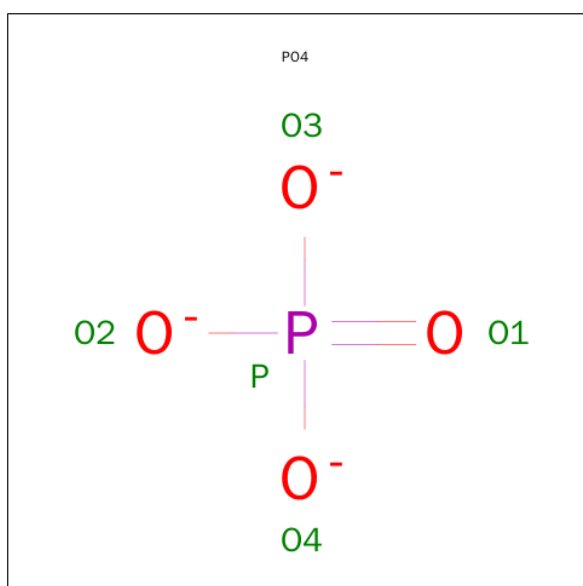
Chain	Residue	Modelled	Actual	Comment	Reference
D	9	MET	-	EXPRESSION TAG	UNP P0C5C1
D	10	GLY	-	EXPRESSION TAG	UNP P0C5C1
D	11	SER	-	EXPRESSION TAG	UNP P0C5C1
D	12	SER	-	EXPRESSION TAG	UNP P0C5C1
D	13	HIS	-	EXPRESSION TAG	UNP P0C5C1
D	14	HIS	-	EXPRESSION TAG	UNP P0C5C1
D	15	HIS	-	EXPRESSION TAG	UNP P0C5C1
D	16	HIS	-	EXPRESSION TAG	UNP P0C5C1
D	17	HIS	-	EXPRESSION TAG	UNP P0C5C1
D	18	HIS	-	EXPRESSION TAG	UNP P0C5C1
D	19	SER	-	EXPRESSION TAG	UNP P0C5C1
D	20	SER	-	EXPRESSION TAG	UNP P0C5C1
D	21	GLY	-	EXPRESSION TAG	UNP P0C5C1
D	22	GLU	-	EXPRESSION TAG	UNP P0C5C1
D	23	ASN	-	EXPRESSION TAG	UNP P0C5C1
D	24	LEU	-	EXPRESSION TAG	UNP P0C5C1
D	25	TYR	-	EXPRESSION TAG	UNP P0C5C1
D	26	PHE	-	EXPRESSION TAG	UNP P0C5C1
D	27	GLN	-	EXPRESSION TAG	UNP P0C5C1
D	28	GLY	-	EXPRESSION TAG	UNP P0C5C1
D	166	ALA	GLU	ENGINEERED MUTATION	UNP P0C5C1

- Molecule 2 is (2R)-2-[(1S)-1-(BENZOYLAMINO)-1-METHOXY-2-OXOETHYL]-5-METHYLIDENE-5,6-DIHYDRO-2H-1,3-THIAZINE-4-CARBOXYLIC ACID (three-letter code: CD8) (formula: C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	16	2	5	1		
2	B	1	Total	C	N	O	S	0	0
			24	16	2	5	1		
2	C	1	Total	C	N	O	S	0	0
			24	16	2	5	1		
2	D	1	Total	C	N	O	S	0	0
			24	16	2	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	3	Total	O	0	0
			3	3		
4	C	4	Total	O	0	0
			4	4		

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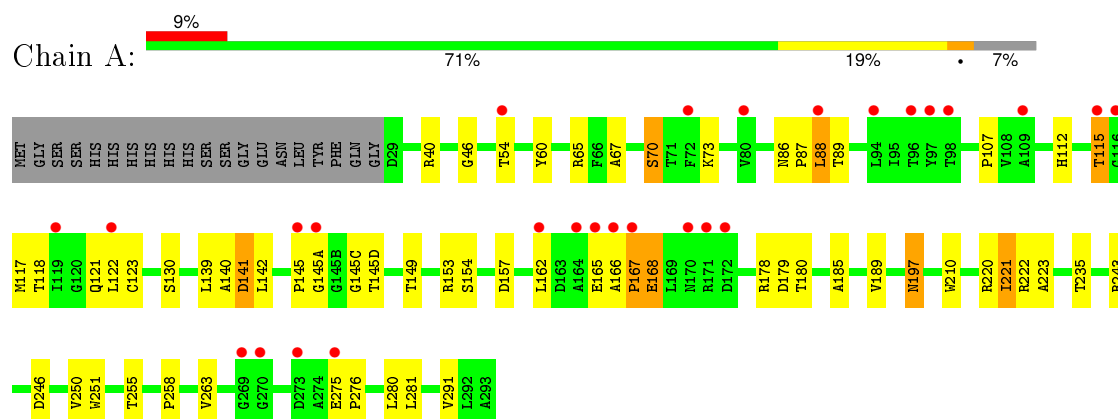
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	O	0	0
			3	3		



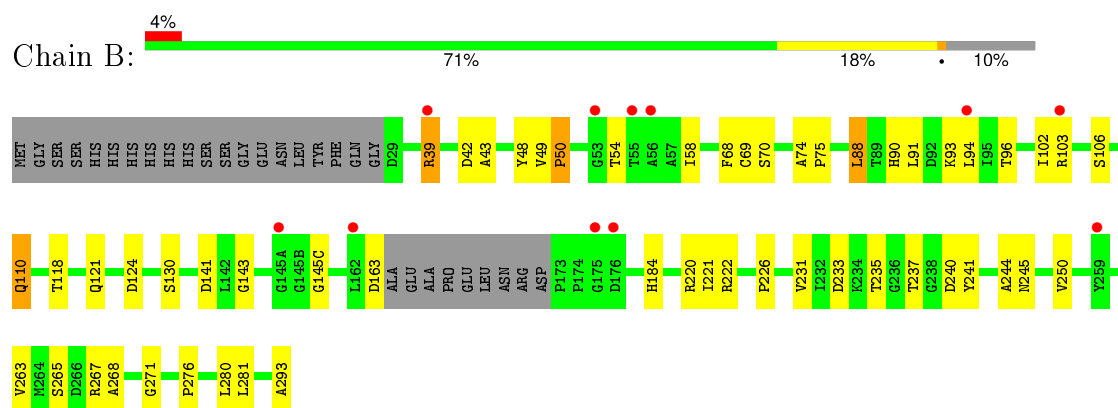
### 3 Residue-property plots

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.

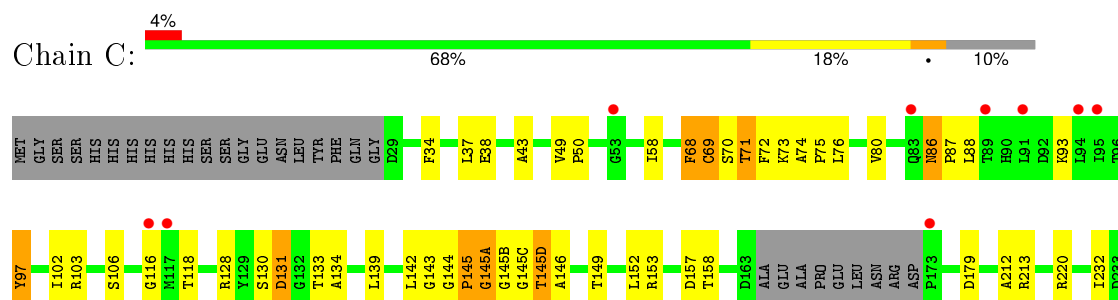
#### • Molecule 1: Beta-lactamase

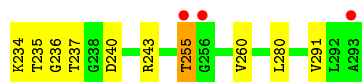


#### • Molecule 1: Beta-lactamase

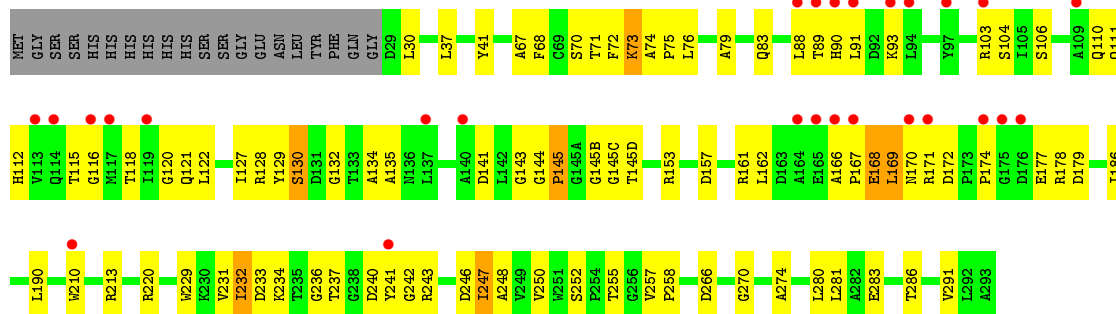


#### • Molecule 1: Beta-lactamase





• Molecule 1: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.06 Å 96.60 Å 108.56 Å 90.00° 107.69° 90.00°	Depositor
Resolution (Å)	47.16 – 2.78 47.16 – 2.78	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.16-2.78) 97.2 (47.16-2.78)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.77 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.245 , 0.260 0.244 , 0.254	Depositor DCC
$R_{free}$ test set	2001 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38864 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7409	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: PO4, CD8

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	0.54	0/1894	0.59	0/2599
1	B	0.49	0/1828	0.65	0/2505
1	C	0.59	0/1832	0.62	0/2513
1	D	0.49	0/1879	0.57	0/2579
All	All	0.53	0/7433	0.61	0/10196

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	1856	0	1738	56	0
1	B	1793	0	1695	58	0
1	C	1795	0	1696	69	0
1	D	1841	0	1710	83	0
2	A	24	0	14	20	0
2	B	24	0	14	22	0
2	C	24	0	14	26	0
2	D	24	0	14	20	0
3	B	5	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
All	All	7409	0	6895	308	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 22.

All (308) 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:B:70:SER:CB	2:B:301:CD8:HACB	1.35	1.52
1:B:70:SER:HB3	2:B:301:CD8:CAC	1.66	1.24
2:A:301:CD8:HACA	2:A:301:CD8:OAG	1.42	1.18
2:C:301:CD8:NAS	2:C:301:CD8:HAO	1.57	1.16
1:B:70:SER:CA	2:B:301:CD8:HACB	1.79	1.13
1:B:39:ARG:HB3	1:B:39:ARG:HH21	1.10	1.06
2:C:301:CD8:OAF	2:C:301:CD8:HAAA	1.56	1.06
2:B:301:CD8:HAAA	2:B:301:CD8:OAF	1.55	1.03
1:B:70:SER:CB	2:B:301:CD8:CAC	2.30	1.02
2:D:301:CD8:HAAA	2:D:301:CD8:OAF	1.55	1.01
2:A:301:CD8:HAO	2:A:301:CD8:HNAS	1.24	1.01
2:A:301:CD8:HAAA	2:A:301:CD8:OAF	1.55	1.01
1:D:70:SER:OG	2:D:301:CD8:HACB	1.66	0.95
2:C:301:CD8:NAS	2:C:301:CD8:CAO	2.29	0.94
1:C:70:SER:HB3	2:C:301:CD8:OAT	1.64	0.94
1:C:240:ASP:O	1:C:243:ARG:HD2	1.67	0.94
1:B:39:ARG:CB	1:B:39:ARG:HH21	1.81	0.93
1:D:220:ARG:HD3	1:D:281:LEU:HD12	1.50	0.92
1:A:70:SER:HB3	1:A:73:LYS:HZ2	1.34	0.91
1:B:70:SER:HB3	2:B:301:CD8:HACB	0.91	0.91
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.01	0.90
1:A:197:ASN:H	1:A:197:ASN:HD22	1.14	0.90
1:D:240:ASP:O	1:D:243:ARG:HG3	1.70	0.89
2:C:301:CD8:HAO	2:C:301:CD8:CAZ	2.03	0.89
2:C:301:CD8:HNAS	2:C:301:CD8:HAO	1.33	0.89
2:C:301:CD8:OAG	2:C:301:CD8:HACA	1.72	0.88
2:D:301:CD8:NAS	2:D:301:CD8:HAO	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:CD8:CAO	2:A:301:CD8:HNAS	1.85	0.87
2:D:301:CD8:HACA	2:D:301:CD8:OAG	1.76	0.86
1:D:237:THR:OG1	2:D:301:CD8:CAA	2.25	0.84
1:B:39:ARG:HB3	1:B:39:ARG:NH2	1.92	0.84
2:C:301:CD8:CAZ	2:C:301:CD8:HACA	2.09	0.82
1:C:74:ALA:HB3	1:C:75:PRO:HD3	1.61	0.82
1:A:145(D):THR:HB	1:A:162:LEU:O	1.80	0.81
1:A:263:VAL:HG12	1:A:281:LEU:HD22	1.62	0.81
1:B:263:VAL:HG12	1:B:281:LEU:HD22	1.62	0.80
1:C:145(A):GLY:O	1:C:145(D):THR:CG2	2.30	0.80
2:D:301:CD8:CAA	2:D:301:CD8:OAF	2.30	0.80
1:C:255:THR:O	1:C:255:THR:CG2	2.30	0.79
1:A:167:PRO:O	1:A:168:GLU:CB	2.31	0.79
2:B:301:CD8:HAM	2:B:301:CD8:HAO	1.65	0.79
1:C:131:ASP:C	1:C:131:ASP:OD1	2.21	0.79
2:C:301:CD8:OAG	2:C:301:CD8:CAC	2.30	0.78
2:B:301:CD8:CAA	2:B:301:CD8:OAF	2.30	0.77
2:C:301:CD8:OAF	2:C:301:CD8:CAA	2.30	0.77
2:C:301:CD8:CAM	2:C:301:CD8:HAO	2.13	0.77
1:D:247:ILE:O	1:D:247:ILE:HG12	1.84	0.76
1:C:70:SER:HB2	1:C:73:LYS:HE3	1.67	0.76
2:A:301:CD8:CAC	2:A:301:CD8:OAG	2.30	0.75
1:C:68:PHE:HB2	1:C:179:ASP:O	1.87	0.75
2:A:301:CD8:NAS	2:A:301:CD8:HAO	2.02	0.75
1:A:70:SER:HB3	2:A:301:CD8:HACB	1.69	0.75
1:C:103:ARG:HA	1:D:110:GLN:HG2	1.67	0.75
1:D:255:THR:O	1:D:255:THR:HG22	1.87	0.74
1:C:145(A):GLY:C	1:C:145(D):THR:HG23	2.08	0.74
1:A:220:ARG:HD3	1:A:281:LEU:HD12	1.70	0.74
1:B:70:SER:CA	2:B:301:CD8:CAC	2.60	0.73
1:C:130:SER:OG	2:C:301:CD8:NAQ	2.21	0.73
2:A:301:CD8:HAO	2:A:301:CD8:HAM	1.70	0.73
1:A:197:ASN:H	1:A:197:ASN:ND2	1.86	0.72
1:D:128:ARG:HD2	1:D:213:ARG:O	1.90	0.72
1:B:220:ARG:NH2	1:B:245:ASN:O	2.23	0.71
1:A:178:ARG:O	1:A:179:ASP:HB2	1.89	0.71
1:D:237:THR:OG1	2:D:301:CD8:HAAA	1.90	0.70
1:C:68:PHE:O	1:C:69:CYS:HB2	1.91	0.69
1:C:255:THR:O	1:C:255:THR:HG22	1.91	0.69
1:B:70:SER:H	2:B:301:CD8:CBA	2.04	0.69
1:B:263:VAL:CG1	1:B:281:LEU:HD22	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:VAL:HG22	1:D:250:VAL:HG12	1.75	0.68
2:C:301:CD8:HAM	2:C:301:CD8:HAO	1.73	0.68
1:C:38:GLU:HG2	1:C:43:ALA:O	1.94	0.68
1:A:139:LEU:O	1:A:140:ALA:C	2.32	0.68
2:D:301:CD8:HNAS	2:D:301:CD8:HAO	1.58	0.68
1:C:220:ARG:NH2	1:C:235:THR:HB	2.09	0.67
2:B:301:CD8:HNAS	2:B:301:CD8:HAO	1.59	0.67
1:C:130:SER:OG	2:C:301:CD8:CBE	2.42	0.67
1:C:70:SER:CB	1:C:73:LYS:HE3	2.25	0.66
1:A:67:ALA:HB3	1:A:243:ARG:HD3	1.75	0.66
1:A:86:ASN:HB3	1:A:87:PRO:HD2	1.78	0.65
1:C:237:THR:N	2:C:301:CD8:OAH	2.22	0.65
1:A:140:ALA:O	1:A:142:LEU:N	2.30	0.65
1:C:145:PRO:O	1:C:145(B):GLY:N	2.30	0.65
1:C:145:PRO:C	1:C:145(B):GLY:H	2.00	0.65
1:C:86:ASN:ND2	1:C:86:ASN:N	2.46	0.64
2:C:301:CD8:HAO	2:C:301:CD8:CBC	2.27	0.64
1:D:167:PRO:O	1:D:168:GLU:C	2.34	0.64
1:D:167:PRO:O	1:D:169:LEU:N	2.30	0.64
1:A:145(A):GLY:O	1:A:145(D):THR:HG23	1.97	0.64
1:A:139:LEU:O	1:A:142:LEU:N	2.30	0.64
1:A:140:ALA:C	1:A:142:LEU:H	2.01	0.64
2:D:301:CD8:CAO	2:D:301:CD8:NAS	2.56	0.63
1:C:131:ASP:OD1	1:C:134:ALA:N	2.22	0.63
1:B:118:THR:H	1:B:121:GLN:NE2	1.96	0.63
1:B:231:VAL:HG22	1:B:250:VAL:HG12	1.81	0.63
1:D:233:ASP:HB3	1:D:248:ALA:HB2	1.81	0.63
1:C:74:ALA:CB	1:C:75:PRO:CD	2.72	0.62
2:C:301:CD8:CAC	2:C:301:CD8:CAZ	2.75	0.62
1:B:48:TYR:CZ	1:B:184:HIS:CD2	2.88	0.62
1:C:149:THR:O	1:C:153:ARG:HG2	1.99	0.62
2:D:301:CD8:CAO	2:D:301:CD8:HNAS	2.11	0.61
1:C:70:SER:HB3	2:C:301:CD8:CAC	2.31	0.61
1:C:74:ALA:HB3	1:C:75:PRO:HD2	1.83	0.60
2:B:301:CD8:HAM	2:B:301:CD8:CAO	2.31	0.60
1:B:70:SER:OG	2:B:301:CD8:NAQ	2.30	0.59
1:C:145(A):GLY:C	1:C:145(D):THR:CG2	2.70	0.59
1:B:70:SER:N	2:B:301:CD8:CBA	2.65	0.59
2:D:301:CD8:CAZ	2:D:301:CD8:HACA	2.32	0.59
1:B:69:CYS:HB3	2:B:301:CD8:OAH	2.02	0.59
2:A:301:CD8:NAS	2:A:301:CD8:CAO	2.63	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PRO:HG3	1:B:110:GLN:OE1	2.03	0.59
1:D:233:ASP:CB	1:D:248:ALA:HB2	2.33	0.58
1:B:106:SER:O	1:B:110:GLN:HB2	2.03	0.58
1:C:86:ASN:HB3	1:C:87:PRO:HD2	1.85	0.58
1:C:128:ARG:HD2	1:C:213:ARG:O	2.03	0.58
2:A:301:CD8:OAF	2:A:301:CD8:CAA	2.30	0.58
1:D:70:SER:HB2	1:D:236:GLY:HA2	1.83	0.58
1:B:70:SER:N	2:B:301:CD8:OAH	2.30	0.58
1:C:143:GLY:O	1:C:145(C):GLY:HA2	2.04	0.58
1:A:70:SER:CB	2:A:301:CD8:HACB	2.31	0.58
1:D:76:LEU:O	1:D:76:LEU:HD12	2.04	0.58
1:D:130:SER:HB3	2:D:301:CD8:HBE	1.86	0.57
1:D:174:PRO:HD3	1:D:241:TYR:CE2	2.38	0.57
1:D:169:LEU:O	1:D:171:ARG:N	2.30	0.57
2:D:301:CD8:OAG	2:D:301:CD8:CAC	2.52	0.57
1:C:145(A):GLY:CA	1:C:145(D):THR:HG23	2.35	0.57
1:C:130:SER:OG	2:C:301:CD8:HBE	2.03	0.57
1:C:145(A):GLY:HA3	1:C:145(D):THR:HG23	1.88	0.56
1:C:49:VAL:HB	1:C:58:ILE:HB	1.86	0.56
1:D:247:ILE:O	1:D:247:ILE:CG1	2.53	0.56
1:B:93:LYS:O	1:B:118:THR:HA	2.06	0.56
2:B:301:CD8:HNAS	2:B:301:CD8:CAO	2.18	0.56
1:B:48:TYR:CE2	1:B:184:HIS:HD2	2.24	0.55
1:A:118:THR:O	1:A:122:LEU:HG	2.07	0.55
1:D:129:TYR:O	1:D:130:SER:CB	2.52	0.55
1:A:185:ALA:O	1:A:189:VAL:HG23	2.06	0.55
2:D:301:CD8:CBA	2:D:301:CD8:OAG	2.54	0.55
1:B:90:HIS:HE1	1:B:141:ASP:OD2	1.90	0.55
1:C:97:TYR:CE2	1:C:116:GLY:HA2	2.42	0.55
1:B:43:ALA:HB2	1:B:267:ARG:HG2	1.90	0.54
1:B:70:SER:HA	2:B:301:CD8:HACB	1.81	0.54
1:D:70:SER:OG	2:D:301:CD8:CAC	2.44	0.54
1:D:130:SER:OG	2:D:301:CD8:NAQ	2.28	0.54
1:A:86:ASN:HB3	1:A:87:PRO:CD	2.38	0.54
1:B:70:SER:N	2:B:301:CD8:CAC	2.71	0.54
1:A:149:THR:O	1:A:153:ARG:HG2	2.08	0.54
1:A:250:VAL:O	1:A:258:PRO:HA	2.07	0.54
1:B:124:ASP:OD2	3:B:302:PO4:O4	2.26	0.53
1:B:124:ASP:OD1	3:B:302:PO4:O4	2.26	0.53
1:B:39:ARG:CG	1:B:39:ARG:HH21	2.21	0.53
1:A:197:ASN:HD22	1:A:197:ASN:N	1.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:SER:OG	1:D:132:GLY:HA3	2.09	0.53
2:A:301:CD8:CAM	2:A:301:CD8:HAO	2.39	0.53
1:D:237:THR:CB	2:D:301:CD8:CAA	2.86	0.53
1:A:220:ARG:O	1:A:221:ILE:C	2.45	0.53
1:C:68:PHE:CE2	1:C:72:PHE:HB3	2.44	0.53
1:B:118:THR:H	1:B:121:GLN:HE21	1.55	0.53
1:C:212:ALA:HA	1:C:232:ILE:HG22	1.90	0.53
1:C:152:LEU:O	1:C:157:ASP:HB3	2.08	0.53
1:D:106:SER:O	1:D:110:GLN:HB2	2.09	0.53
1:B:48:TYR:CZ	1:B:184:HIS:HD2	2.27	0.52
1:A:130:SER:OG	2:A:301:CD8:NAQ	2.37	0.52
1:D:255:THR:O	1:D:255:THR:CG2	2.54	0.52
1:D:190:LEU:HD22	1:D:247:ILE:HG13	1.92	0.52
1:B:124:ASP:CG	3:B:302:PO4:O4	2.47	0.52
1:D:167:PRO:C	1:D:169:LEU:N	2.61	0.52
2:C:301:CD8:CAZ	2:C:301:CD8:CAO	2.82	0.52
1:D:240:ASP:C	1:D:242:GLY:N	2.63	0.52
1:A:145(A):GLY:C	1:A:145(C):GLY:H	2.13	0.52
1:C:131:ASP:OD1	1:C:133:THR:N	2.43	0.51
1:D:73:LYS:HD3	1:D:135:ALA:HB2	1.92	0.51
1:D:161:ARG:HD3	1:D:177:GLU:O	2.10	0.51
1:D:30:LEU:HD22	1:D:291:VAL:HG21	1.92	0.51
1:C:93:LYS:O	1:C:118:THR:HA	2.11	0.51
1:D:118:THR:H	1:D:121:GLN:NE2	2.09	0.51
1:C:255:THR:O	1:C:255:THR:HG23	2.10	0.51
1:A:140:ALA:C	1:A:142:LEU:N	2.64	0.50
1:A:118:THR:H	1:A:121:GLN:NE2	2.09	0.50
1:B:49:VAL:O	1:B:50:PRO:O	2.30	0.50
1:C:144:GLY:O	1:C:145:PRO:O	2.30	0.50
1:C:131:ASP:CG	1:C:134:ALA:H	2.12	0.50
1:C:145:PRO:C	1:C:145(B):GLY:N	2.65	0.50
1:D:68:PHE:O	1:D:71:THR:OG1	2.30	0.49
1:A:165:GLU:O	1:A:167:PRO:O	2.30	0.49
1:D:144:GLY:O	1:D:145:PRO:O	2.30	0.49
1:C:58:ILE:HD11	1:C:291:VAL:HG11	1.94	0.49
1:C:220:ARG:HH21	1:C:235:THR:HB	1.77	0.49
1:A:65:ARG:NH1	1:A:180:THR:OG1	2.44	0.49
2:A:301:CD8:OAH	2:A:301:CD8:OAG	2.30	0.49
1:D:168:GLU:O	1:D:169:LEU:O	2.30	0.49
1:A:141:ASP:OD2	1:A:141:ASP:O	2.30	0.49
1:D:122:LEU:HD22	1:D:134:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:CD8:HACA	2:A:301:CD8:CAZ	2.34	0.49
1:D:233:ASP:OD2	1:D:246:ASP:OD1	2.30	0.49
1:B:49:VAL:O	1:B:50:PRO:C	2.50	0.49
1:B:70:SER:N	2:B:301:CD8:HACB	2.26	0.49
1:A:73:LYS:NZ	2:A:301:CD8:CAC	2.76	0.49
1:A:220:ARG:O	1:A:222:ARG:N	2.46	0.48
1:C:145(C):GLY:C	1:C:146:ALA:H	2.16	0.48
2:C:301:CD8:OAG	2:C:301:CD8:OAT	2.30	0.48
1:D:79:ALA:O	1:D:83:GLN:HG3	2.14	0.48
1:B:244:ALA:HB2	1:B:276:PRO:HB3	1.95	0.48
2:C:301:CD8:HNAS	2:C:301:CD8:CAO	2.09	0.48
1:C:97:TYR:CD2	1:C:97:TYR:N	2.82	0.48
1:B:241:TYR:HB3	1:B:268:ALA:HA	1.96	0.48
1:B:70:SER:HA	2:B:301:CD8:CAC	2.42	0.48
1:A:117:MET:HB2	1:A:122:LEU:HD21	1.95	0.48
1:C:50:PRO:HD2	1:C:260:VAL:O	2.14	0.47
1:D:129:TYR:O	1:D:130:SER:HB2	2.14	0.47
1:B:143:GLY:O	1:B:145(C):GLY:HA2	2.14	0.47
1:C:58:ILE:HD11	1:C:291:VAL:CG1	2.45	0.47
1:D:91:LEU:HD22	1:D:120:GLY:HA2	1.96	0.47
1:D:112:HIS:CD2	1:D:115:THR:HG21	2.50	0.47
1:B:220:ARG:O	1:B:221:ILE:C	2.53	0.47
1:D:153:ARG:HD3	1:D:157:ASP:O	2.13	0.47
2:A:301:CD8:CAZ	2:A:301:CD8:OAH	2.62	0.47
1:D:232:ILE:O	1:D:248:ALA:HB1	2.15	0.47
1:A:251:TRP:NE1	1:A:258:PRO:HB3	2.30	0.47
1:B:241:TYR:HA	1:B:271:GLY:O	2.15	0.47
1:A:255:THR:O	1:A:255:THR:CG2	2.63	0.47
1:A:263:VAL:CG1	1:A:281:LEU:HD22	2.40	0.46
1:C:145(A):GLY:O	1:C:145(D):THR:HG21	2.12	0.46
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.71	0.46
1:A:141:ASP:CG	1:A:141:ASP:O	2.53	0.46
1:A:112:HIS:HD2	1:A:115:THR:HG21	1.81	0.46
1:C:86:ASN:H	1:C:86:ASN:HD22	1.64	0.46
1:C:145(C):GLY:C	1:C:146:ALA:N	2.67	0.46
1:C:237:THR:O	2:C:301:CD8:CAM	2.63	0.46
1:B:293:ALA:HB2	1:D:286:THR:CG2	2.46	0.46
1:C:70:SER:HA	1:C:72:PHE:CE2	2.51	0.46
1:C:86:ASN:N	1:C:86:ASN:HD22	2.14	0.45
1:D:67:ALA:O	1:D:68:PHE:C	2.53	0.45
1:D:229:TRP:CE3	1:D:252:SER:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:SER:OG	2:A:301:CD8:HBE	2.17	0.45
1:C:73:LYS:HB2	1:C:234:LYS:HE2	1.97	0.45
1:D:93:LYS:O	1:D:118:THR:HA	2.17	0.45
1:C:236:GLY:HA2	2:C:301:CD8:OAH	2.17	0.45
1:A:197:ASN:N	1:A:197:ASN:ND2	2.53	0.45
1:D:104:SER:OG	1:D:166:ALA:HB1	2.16	0.45
1:C:72:PHE:HD2	1:C:72:PHE:H	1.63	0.45
1:B:220:ARG:HD3	1:B:281:LEU:HD12	1.98	0.45
1:D:72:PHE:HE1	1:D:76:LEU:HD22	1.82	0.45
1:B:49:VAL:HB	1:B:58:ILE:HB	1.99	0.45
1:C:68:PHE:O	1:C:71:THR:OG1	2.30	0.44
1:C:70:SER:H	2:C:301:CD8:CBA	2.30	0.44
1:D:76:LEU:O	1:D:79:ALA:HB3	2.17	0.44
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.71	0.44
1:B:240:ASP:O	1:B:241:TYR:HB2	2.18	0.44
1:B:293:ALA:C	1:D:283:GLU:OE1	2.56	0.44
1:D:103:ARG:CB	1:D:167:PRO:HD3	2.48	0.44
1:D:145:PRO:C	1:D:145(B):GLY:H	2.21	0.44
1:A:153:ARG:HD3	1:A:157:ASP:O	2.18	0.44
1:D:111:GLN:O	1:D:112:HIS:ND1	2.51	0.44
1:B:39:ARG:CB	1:B:39:ARG:NH2	2.65	0.44
1:D:72:PHE:C	1:D:72:PHE:CD1	2.91	0.44
1:C:72:PHE:O	1:C:75:PRO:HD2	2.18	0.43
1:C:72:PHE:O	1:C:75:PRO:CD	2.66	0.43
1:D:240:ASP:O	1:D:242:GLY:N	2.52	0.43
1:D:229:TRP:CD2	1:D:252:SER:HA	2.54	0.43
1:B:88:LEU:O	1:B:91:LEU:HG	2.18	0.43
1:A:46:GLY:HA2	1:A:60:TYR:O	2.19	0.43
1:D:37:LEU:O	1:D:41:TYR:HD1	2.01	0.43
1:D:90:HIS:HE1	1:D:141:ASP:OD2	2.01	0.43
1:A:70:SER:OG	2:A:301:CD8:NAQ	2.51	0.43
1:C:69:CYS:O	1:C:72:PHE:CD2	2.71	0.43
1:D:257:VAL:HA	1:D:258:PRO:HD3	1.88	0.43
1:D:127:ILE:HG21	1:D:210:TRP:HB3	2.00	0.42
1:D:178:ARG:O	1:D:179:ASP:HB2	2.19	0.42
1:A:275:GLU:HA	1:A:276:PRO:HD3	1.91	0.42
1:A:220:ARG:O	1:A:223:ALA:N	2.45	0.42
1:D:143:GLY:O	1:D:145(C):GLY:HA2	2.18	0.42
1:C:76:LEU:O	1:C:76:LEU:HD12	2.18	0.42
1:D:70:SER:O	1:D:234:LYS:HE3	2.18	0.42
1:A:117:MET:HA	1:A:121:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145(D):THR:HB	1:D:162:LEU:O	2.19	0.42
1:C:34:PHE:O	1:C:37:LEU:HB2	2.18	0.42
1:D:240:ASP:O	1:D:241:TYR:C	2.57	0.42
1:A:235:THR:HG22	1:A:246:ASP:OD1	2.20	0.42
1:C:139:LEU:O	1:C:142:LEU:HB2	2.19	0.42
1:A:73:LYS:HZ1	2:A:301:CD8:CAC	2.33	0.42
1:B:74:ALA:HB3	1:B:75:PRO:HD2	2.01	0.42
1:B:220:ARG:HD2	1:B:235:THR:HG22	2.02	0.41
1:D:168:GLU:O	1:D:169:LEU:C	2.58	0.41
1:D:270:GLY:HA3	1:D:274:ALA:HB2	2.02	0.41
1:B:70:SER:N	2:B:301:CD8:HACA	2.35	0.41
1:D:237:THR:HB	2:D:301:CD8:CAA	2.51	0.41
1:D:166:ALA:HA	1:D:167:PRO:HA	1.56	0.41
1:A:123:CYS:HB3	1:A:210:TRP:CZ3	2.55	0.41
1:C:80:VAL:O	1:C:86:ASN:ND2	2.54	0.41
1:D:233:ASP:HB3	1:D:248:ALA:CB	2.48	0.41
1:B:222:ARG:NH2	1:B:226:PRO:O	2.53	0.41
1:B:94:LEU:HA	1:B:94:LEU:HD12	1.85	0.41
1:D:240:ASP:C	1:D:242:GLY:H	2.22	0.41
1:A:263:VAL:HG12	1:A:281:LEU:CD2	2.41	0.41
1:D:130:SER:HB3	2:D:301:CD8:CBE	2.51	0.41
1:D:115:THR:HG23	1:D:116:GLY:O	2.21	0.41
1:A:88:LEU:HA	1:A:88:LEU:HD12	1.57	0.41
1:D:172:ASP:O	1:D:241:TYR:CE1	2.74	0.41
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.87	0.41
1:D:74:ALA:HB3	1:D:75:PRO:CD	2.51	0.41
1:A:70:SER:HB3	1:A:73:LYS:NZ	2.18	0.41
1:D:174:PRO:HD3	1:D:241:TYR:CD2	2.57	0.41
1:A:145(A):GLY:C	1:A:145(C):GLY:N	2.74	0.40
1:A:166:ALA:HA	1:A:167:PRO:HA	1.54	0.40
2:C:301:CD8:CAM	2:C:301:CD8:CAO	2.93	0.40
1:D:242:GLY:O	1:D:266:ASP:HA	2.21	0.40
1:B:220:ARG:NH1	1:B:237:THR:OG1	2.36	0.40
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.51	0.40
1:D:130:SER:CB	2:D:301:CD8:NAQ	2.84	0.40

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	263/285 (92%)	245 (93%)	13 (5%)	5 (2%)	10	30
1	B	252/285 (88%)	242 (96%)	9 (4%)	1 (0%)	39	73
1	C	252/285 (88%)	232 (92%)	17 (7%)	3 (1%)	16	44
1	D	263/285 (92%)	240 (91%)	19 (7%)	4 (2%)	13	37
All	All	1030/1140 (90%)	959 (93%)	58 (6%)	13 (1%)	15	41

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	PRO
1	D	145	PRO
1	D	169	LEU
1	A	141	ASP
1	A	168	GLU
1	C	145(A)	GLY
1	D	170	ASN
1	B	50	PRO
1	D	168	GLU
1	A	167	PRO
1	C	69	CYS
1	A	145	PRO
1	A	221	ILE

### 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	166/218 (76%)	156 (94%)	10 (6%)	24	54
1	B	161/218 (74%)	147 (91%)	14 (9%)	13	33
1	C	161/218 (74%)	149 (92%)	12 (8%)	17	40
1	D	162/218 (74%)	155 (96%)	7 (4%)	35	69
All	All	650/872 (74%)	607 (93%)	43 (7%)	21	48

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	54	THR
1	A	70	SER
1	A	88	LEU
1	A	89	THR
1	A	115	THR
1	A	154	SER
1	A	197	ASN
1	A	280	LEU
1	A	291	VAL
1	B	39	ARG
1	B	42	ASP
1	B	54	THR
1	B	68	PHE
1	B	88	LEU
1	B	96	THR
1	B	102	ILE
1	B	103	ARG
1	B	110	GLN
1	B	130	SER
1	B	163	ASP
1	B	233	ASP
1	B	265	SER
1	B	280	LEU
1	C	68	PHE
1	C	71	THR
1	C	86	ASN
1	C	88	LEU
1	C	97	TYR
1	C	102	ILE
1	C	106	SER
1	C	131	ASP
1	C	145(D)	THR

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Mol	Chain	Res	Type
1	C	158	THR
1	C	255	THR
1	C	280	LEU
1	D	73	LYS
1	D	89	THR
1	D	130	SER
1	D	186	ILE
1	D	232	ILE
1	D	247	ILE
1	D	280	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	192	GLN
1	A	197	ASN
1	B	90	HIS
1	B	121	GLN
1	B	184	HIS
1	B	192	GLN
1	C	86	ASN
1	C	90	HIS
1	C	192	GLN
1	D	90	HIS
1	D	121	GLN
1	D	192	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CD8	A	301	1	16,25,25	2.75	3 (18%)	14,35,35	3.44	3 (21%)
2	CD8	B	301	1	16,25,25	2.69	4 (25%)	14,35,35	3.30	3 (21%)
3	PO4	B	302	-	4,4,4	2.02	3 (75%)	6,6,6	0.27	0
2	CD8	C	301	1	16,25,25	2.70	3 (18%)	14,35,35	1.80	2 (14%)
3	PO4	C	302	-	4,4,4	2.02	3 (75%)	6,6,6	0.27	0
2	CD8	D	301	1	16,25,25	2.46	3 (18%)	14,35,35	2.24	1 (7%)
3	PO4	D	302	-	4,4,4	2.01	3 (75%)	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CD8	A	301	1	-	0/6/38/38	0/1/2/2
2	CD8	B	301	1	-	0/6/38/38	0/1/2/2
3	PO4	B	302	-	-	0/0/0/0	0/0/0/0
2	CD8	C	301	1	-	0/6/38/38	0/1/2/2
3	PO4	C	302	-	-	0/0/0/0	0/0/0/0
2	CD8	D	301	1	-	0/6/38/38	0/1/2/2
3	PO4	D	302	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CD8	CAY-CBB	-8.87	1.37	1.52
2	C	301	CD8	CAY-CBB	-8.64	1.37	1.52
2	B	301	CD8	CAY-CBB	-8.61	1.37	1.52
2	D	301	CD8	CAY-CBB	-7.49	1.39	1.52
2	A	301	CD8	CBC-CAZ	-5.49	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	CD8	CBC-CAZ	-5.35	1.38	1.50
2	B	301	CD8	CBC-CAZ	-5.22	1.39	1.50
2	D	301	CD8	CBC-CAZ	-5.07	1.39	1.50
2	B	301	CD8	CBB-CAX	-2.01	1.38	1.45
3	B	302	PO4	P-O1	2.06	1.61	1.52
3	C	302	PO4	P-O1	2.07	1.61	1.52
3	D	302	PO4	P-O1	2.08	1.61	1.52
3	C	302	PO4	P-O2	2.22	1.61	1.53
3	D	302	PO4	P-O2	2.23	1.61	1.53
3	D	302	PO4	P-O3	2.23	1.61	1.53
3	B	302	PO4	P-O2	2.25	1.61	1.53
3	B	302	PO4	P-O3	2.26	1.61	1.53
3	C	302	PO4	P-O3	2.27	1.61	1.53
2	A	301	CD8	CAA-CAX	2.37	1.38	1.32
2	B	301	CD8	CAA-CAX	2.50	1.38	1.32
2	C	301	CD8	CAA-CAX	2.67	1.38	1.32
2	D	301	CD8	CAA-CAX	2.90	1.39	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CD8	CAC-OAT-CBF	-12.19	106.84	114.79
2	B	301	CD8	CAC-OAT-CBF	-10.99	107.62	114.79
2	D	301	CD8	CAC-OAT-CBF	-8.07	109.53	114.79
2	C	301	CD8	CAC-OAT-CBF	-5.48	111.22	114.79
2	B	301	CD8	CBC-CAZ-NAS	-2.29	112.77	117.18
2	A	301	CD8	CBC-CAZ-NAS	-2.11	113.13	117.18
2	C	301	CD8	CAO-SAV-CBE	2.94	99.92	94.37
2	A	301	CD8	CAO-SAV-CBE	3.08	100.18	94.37
2	B	301	CD8	CAO-SAV-CBE	4.45	102.78	94.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CD8	20	0
2	B	301	CD8	22	0
3	B	302	PO4	3	0
2	C	301	CD8	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	CD8	20	0

## 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	265/285 (92%)	0.58	27 (10%) 9 5	54, 71, 103, 125	0
1	B	256/285 (89%)	0.30	11 (4%) 39 31	53, 66, 92, 126	0
1	C	256/285 (89%)	0.37	12 (4%) 35 27	51, 69, 99, 121	0
1	D	265/285 (92%)	0.66	27 (10%) 9 5	56, 72, 107, 123	0
All	All	1042/1140 (91%)	0.48	77 (7%) 17 11	51, 69, 101, 126	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	ALA	7.4
1	A	170	ASN	6.0
1	B	162	LEU	4.8
1	A	97	TYR	4.7
1	B	145(A)	GLY	4.5
1	D	119	ILE	4.5
1	A	164	ALA	4.4
1	B	103	ARG	4.3
1	C	94	LEU	4.3
1	C	116	GLY	4.0
1	D	116	GLY	3.9
1	D	175	GLY	3.8
1	D	88	LEU	3.8
1	D	164	ALA	3.8
1	D	170	ASN	3.7
1	C	293	ALA	3.7
1	D	165	GLU	3.6
1	D	117	MET	3.6
1	D	137	LEU	3.5
1	D	166	ALA	3.5
1	B	176	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	165	GLU	3.4
1	D	113	VAL	3.4
1	A	109	ALA	3.3
1	D	94	LEU	3.3
1	D	210	TRP	3.3
1	A	115	THR	3.2
1	A	167	PRO	3.2
1	C	117	MET	3.2
1	A	96	THR	3.2
1	A	171	ARG	3.2
1	C	53	GLY	3.2
1	D	103	ARG	3.1
1	C	91	LEU	3.1
1	C	256	GLY	3.1
1	A	275	GLU	3.0
1	C	95	ILE	3.0
1	D	90	HIS	3.0
1	A	270	GLY	3.0
1	A	98	THR	2.9
1	A	273	ASP	2.9
1	B	175	GLY	2.9
1	B	53	GLY	2.8
1	D	167	PRO	2.8
1	D	91	LEU	2.6
1	D	174	PRO	2.6
1	D	89	THR	2.6
1	A	72	PHE	2.6
1	A	54	THR	2.5
1	D	241	TYR	2.5
1	A	162	LEU	2.5
1	A	80	VAL	2.5
1	A	94	LEU	2.4
1	C	173	PRO	2.4
1	A	122	LEU	2.4
1	D	114	GLN	2.4
1	A	116	GLY	2.4
1	C	89	THR	2.4
1	D	171	ARG	2.4
1	A	269	GLY	2.4
1	A	172	ASP	2.3
1	D	93	LYS	2.3
1	A	145(A)	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	176	ASP	2.3
1	A	145	PRO	2.3
1	D	140	ALA	2.3
1	D	97	TYR	2.3
1	B	39	ARG	2.2
1	B	56	ALA	2.2
1	B	94	LEU	2.1
1	A	88	LEU	2.1
1	B	259	TYR	2.1
1	D	109	ALA	2.1
1	B	55	THR	2.1
1	C	255	THR	2.1
1	A	119	ILE	2.1
1	C	83	GLN	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	CD8	C	301	24/24	0.77	0.36	5.42	93,102,110,115	0
2	CD8	B	301	24/24	0.82	0.30	2.35	88,95,108,109	0
2	CD8	A	301	24/24	0.88	0.27	0.47	77,87,94,100	0
2	CD8	D	301	24/24	0.89	0.23	0.35	76,86,98,102	0
3	PO4	C	302	5/5	0.91	0.16	-	96,100,115,120	0
3	PO4	D	302	5/5	0.82	0.25	-	92,104,116,120	0
3	PO4	B	302	5/5	0.90	0.12	-	85,90,95,102	0

## 6.5 Other polymers

There are no such residues in this entry.