



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:33 AM UTC

PDB ID : 3VFF / pdb_00003vff
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

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

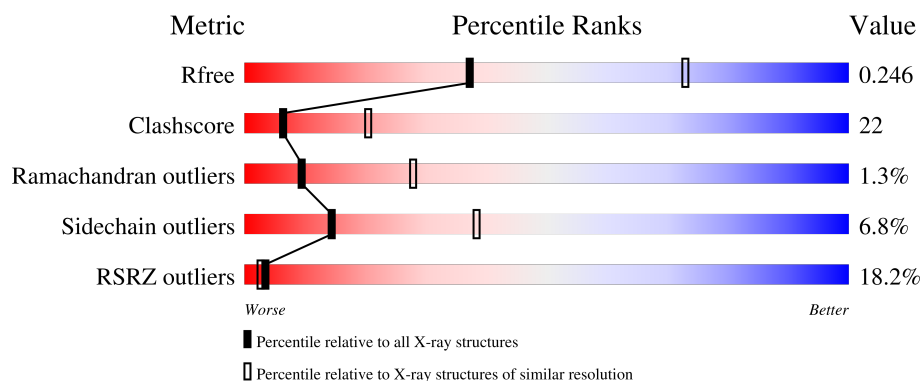
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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 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	285	18% 71% 19% • 7%
1	B	285	15% 72% 16% • 10%
1	C	285	16% 67% 19% • 10%
1	D	285	17% 59% 31% • 7%

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	-
2	CD8	C	301	-	-	X	-
2	CD8	D	301	-	-	X	-
3	PO4	B	302	-	X	X	-
3	PO4	C	302	-	X	-	-
3	PO4	D	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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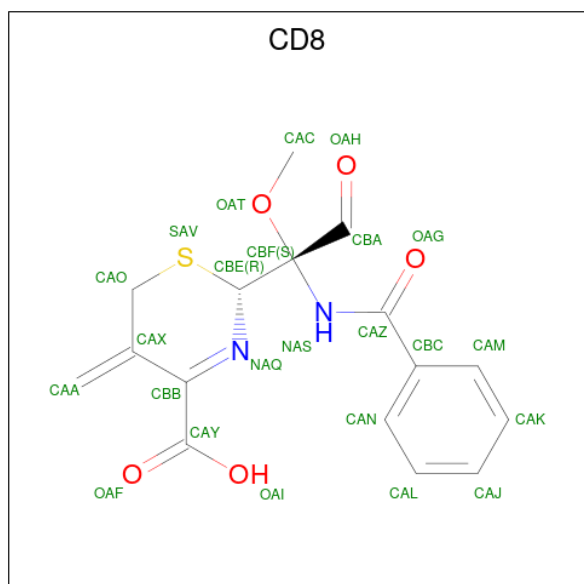
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP P0C5C1
B	10	GLY	-	expression tag	UNP P0C5C1
B	11	SER	-	expression tag	UNP P0C5C1
B	12	SER	-	expression tag	UNP P0C5C1
B	13	HIS	-	expression tag	UNP P0C5C1
B	14	HIS	-	expression tag	UNP P0C5C1
B	15	HIS	-	expression tag	UNP P0C5C1
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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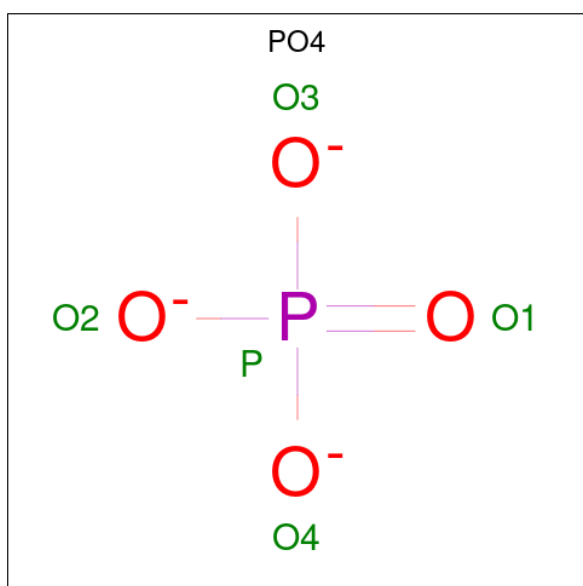
Chain	Residue	Modelled	Actual	Comment	Reference
D	9	MET	-	expression tag	UNP P0C5C1
D	10	GLY	-	expression tag	UNP P0C5C1
D	11	SER	-	expression tag	UNP P0C5C1
D	12	SER	-	expression tag	UNP P0C5C1
D	13	HIS	-	expression tag	UNP P0C5C1
D	14	HIS	-	expression tag	UNP P0C5C1
D	15	HIS	-	expression tag	UNP P0C5C1
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 (CCD ID: CD8) (formula: C₁₆H₁₆N₂O₅S).



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 (CCD ID: PO4) (formula: O₄P).



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			

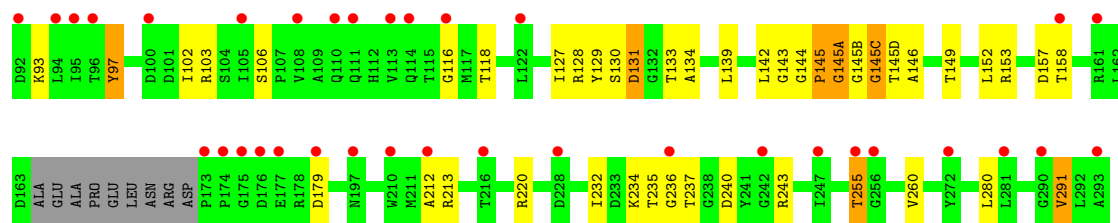
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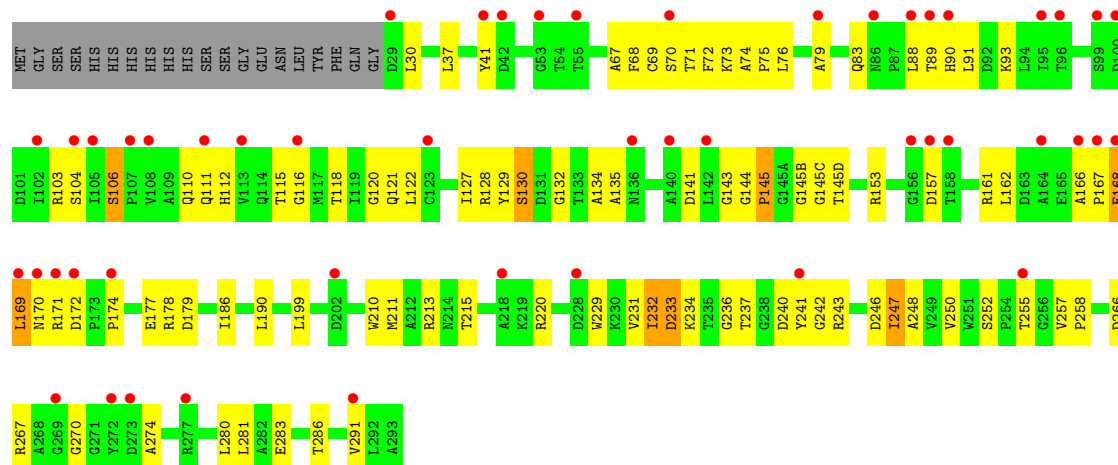
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	O	0	0
			3	3		

- 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, α , β , γ	80.06Å 96.60Å 108.56Å 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) 97.3 (47.16-2.78)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.245 , 0.260 0.239 , 0.246	Depositor DCC
R_{free} test set	2001 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	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	0.92	EDS
Total number of atoms	7409	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CD8, PO4

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	0.75	0/1894	0.89	0/2599
1	B	0.67	0/1828	0.96	2/2505 (0.1%)
1	C	0.88	0/1832	0.94	2/2513 (0.1%)
1	D	0.70	0/1879	0.95	5/2579 (0.2%)
All	All	0.75	0/7433	0.94	9/10196 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	LEU	CA-C-N	7.75	125.24	119.66
1	D	199	LEU	C-N-CA	7.75	125.24	119.66
1	D	233	ASP	N-CA-C	6.75	117.50	108.38
1	B	144	GLY	CA-C-N	6.44	126.42	119.78
1	B	144	GLY	C-N-CA	6.44	126.42	119.78
1	C	145(C)	GLY	N-CA-C	-5.71	107.18	114.37
1	C	127	ILE	N-CA-C	5.42	115.63	110.53
1	D	106	SER	CA-C-N	5.09	124.80	119.82
1	D	106	SER	C-N-CA	5.09	124.80	119.82

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	1856	0	1738	57	0
1	B	1793	0	1695	58	0
1	C	1795	0	1696	71	0
1	D	1841	0	1710	86	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
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	314	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 (314) 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:HH21	1:B:39:ARG:HB3	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:OAF	2:A:301:CD8:HAAA	1.55	1.01
1:D:70:SER:OG	2:D:301:CD8:HACB	1.66	0.95
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
2:C:301:CD8:NAS	2:C:301:CD8:CAO	2.29	0.94
1:B:39:ARG:HH21	1:B:39:ARG:CB	1.81	0.93
1:D:220:ARG:HD3	1:D:281:LEU:HD12	1.50	0.92
1:B:70:SER:HB3	2:B:301:CD8:HACB	0.91	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.01	0.90
1:A:197:ASN:HD22	1:A:197:ASN:H	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:HAO	2:C:301:CD8:HNAS	1.33	0.89
2:C:301:CD8:OAG	2:C:301:CD8:HACA	1.72	0.88
2:D:301:CD8:HAO	2:D:301:CD8:NAS	1.89	0.87
2:A:301:CD8:HNAS	2:A:301:CD8:CAO	1.85	0.87
2:D:301:CD8:OAG	2:D:301:CD8:HACA	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
1:C:131:ASP:OD1	1:C:131:ASP:C	2.21	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:73:LYS:HZ2	2:A:301:CD8:CAC	1.93	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:OAF	2:D:301:CD8:CAA	2.30	0.80
1:C:255:THR:CG2	1:C:255:THR:O	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:145(A):GLY:C	1:C:145(D):THR:HG23	2.08	0.79
2:C:301:CD8:OAG	2:C:301:CD8:CAC	2.30	0.78
2:B:301:CD8:OAF	2:B:301:CD8:CAA	2.30	0.77
2:C:301:CD8:OAF	2:C:301:CD8:CAA	2.30	0.77
2:C:301:CD8:HAO	2:C:301:CD8:CAM	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:OAG	2:A:301:CD8:CAC	2.30	0.75
1:C:68:PHE:HB2	1:C:179:ASP:O	1.87	0.75
2:A:301:CD8:HAO	2:A:301:CD8:NAS	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:HG22	1:D:255:THR:O	1.87	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:139:LEU:O	1:A:140:ALA:C	2.32	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:PRO:C	1:C:145(B):GLY:H	2.00	0.69
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:D:167:PRO:O	1:D:168:GLU:C	2.34	0.69
1:B:263:VAL:CG1	1:B:281:LEU:HD22	2.23	0.68
1:A:140:ALA:C	1:A:142:LEU:H	2.01	0.68
1:D:231:VAL:HG22	1:D:250:VAL:HG12	1.75	0.68
1:C:38:GLU:HG2	1:C:43:ALA:O	1.94	0.68
2:C:301:CD8:HAO	2:C:301:CD8:HAM	1.73	0.68
2:D:301:CD8:HAO	2:D:301:CD8:HNAS	1.58	0.68
1:C:220:ARG:NH2	1:C:235:THR:HB	2.09	0.67
2:B:301:CD8:HAO	2:B:301:CD8:HNAS	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:A:140:ALA:O	1:A:142:LEU:N	2.30	0.65
1:C:237:THR:N	2:C:301:CD8:OAH	2.22	0.65
1:C:145:PRO:O	1:C:145(B):GLY:N	2.30	0.65
1:C:86:ASN:N	1:C:86:ASN:ND2	2.46	0.64
1:C:145(A):GLY:C	1:C:145(D):THR:CG2	2.70	0.64
2:C:301:CD8:HAO	2:C:301:CD8:CBC	2.27	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
2:D:301:CD8:NAS	2:D:301:CD8:CAO	2.56	0.63
1:B:118:THR:H	1:B:121:GLN:NE2	1.96	0.63
1:C:131:ASP:OD1	1:C:134:ALA:N	2.22	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
1:B:48:TYR:CZ	1:B:184:HIS:CD2	2.88	0.62
2:C:301:CD8:CAZ	2:C:301:CD8:CAC	2.75	0.62
1:C:149:THR:O	1:C:153:ARG:HG2	1.99	0.62
2:D:301:CD8:HNAS	2:D:301:CD8:CAO	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:70:SER:N	2:B:301:CD8:CBA	2.65	0.59
2:D:301:CD8:HACA	2:D:301:CD8:CAZ	2.32	0.59
1:B:69:CYS:HB3	2:B:301:CD8:OAH	2.02	0.59
2:A:301:CD8:CAO	2:A:301:CD8:NAS	2.63	0.59
1:D:130:SER:OG	2:D:301:CD8:NAQ	2.28	0.59
1:A:107:PRO:HG3	1:B:110:GLN:OE1	2.03	0.59
1:B:106:SER:O	1:B:110:GLN:HB2	2.03	0.58
1:D:233:ASP:CB	1:D:248:ALA:HB2	2.33	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:HB3	1:A:73:LYS:NZ	2.18	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:A:220:ARG:O	1:A:221:ILE:C	2.45	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:B:124:ASP:CG	3:B:302:PO4:O4	2.47	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:D:167:PRO:C	1:D:169:LEU:N	2.61	0.57
1:C:49:VAL:HB	1:C:58:ILE:HB	1.86	0.56
1:C:145(A):GLY:HA3	1:C:145(D):THR:HG23	1.88	0.56
1:A:145(A):GLY:C	1:A:145(C):GLY:H	2.13	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:A:118:THR:O	1:A:122:LEU:HG	2.07	0.55
1:B:48:TYR:CE2	1:B:184:HIS:HD2	2.24	0.55
1:A:185:ALA:O	1:A:189:VAL:HG23	2.06	0.55
1:D:129:TYR:O	1:D:130:SER:CB	2.52	0.55
1:B:90:HIS:HE1	1:B:141:ASP:OD2	1.90	0.55
2:D:301:CD8:OAG	2:D:301:CD8:CBA	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:131:ASP:CG	1:C:134:ALA:H	2.12	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:A:86:ASN:HB3	1:A:87:PRO:CD	2.38	0.54
1:A:149:THR:O	1:A:153:ARG:HG2	2.08	0.54
1:B:70:SER:N	2:B:301:CD8:CAC	2.71	0.54
1:C:145(C):GLY:C	1:C:146:ALA:H	2.16	0.54
1:A:250:VAL:O	1:A:258:PRO:HA	2.07	0.54
1:B:49:VAL:O	1:B:50:PRO:C	2.50	0.53
1:B:124:ASP:OD2	3:B:302:PO4:O4	2.26	0.53
1:D:190:LEU:HD11	1:D:211:MET:HE1	1.91	0.53
1:D:240:ASP:C	1:D:242:GLY:N	2.63	0.53
1:B:124:ASP:OD1	3:B:302:PO4:O4	2.26	0.53
1:A:197:ASN:HD22	1:A:197:ASN:N	1.86	0.53
1:B:39:ARG:HH21	1:B:39:ARG:CG	2.21	0.53
1:D:104:SER:OG	1:D:132:GLY:HA3	2.09	0.53
2:A:301:CD8:HAO	2:A:301:CD8:CAM	2.39	0.53
1:D:237:THR:CB	2:D:301:CD8:CAA	2.86	0.53
1:B:118:THR:H	1:B:121:GLN:HE21	1.55	0.53
1:C:68:PHE:CE2	1:C:72:PHE:HB3	2.44	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:220:ARG:O	1:B:221:ILE:C	2.53	0.52
2:C:301:CD8:CAO	2:C:301:CD8:CAZ	2.82	0.52
1:A:73:LYS:HZ2	2:A:301:CD8:HACB	1.73	0.51
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:30:LEU:HD22	1:D:291:VAL:HG21	1.92	0.51
1:D:161:ARG:HD3	1:D:177:GLU:O	2.10	0.51
1:A:141:ASP:CG	1:A:141:ASP:O	2.53	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:D:247:ILE:O	1:D:247:ILE:CG1	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:H	1:A:121:GLN:NE2	2.09	0.50
1:C:145(C):GLY:C	1:C:146:ALA:N	2.67	0.50
1:B:49:VAL:O	1:B:50:PRO:O	2.30	0.50
1:D:67:ALA:O	1:D:68:PHE:C	2.53	0.50
1:C:144:GLY:O	1:C:145:PRO:O	2.30	0.50
1:A:70:SER:HB3	1:A:73:LYS:HZ2	1.75	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:A:65:ARG:NH1	1:A:180:THR:OG1	2.44	0.49
1:C:220:ARG:HH21	1:C:235:THR:HB	1.77	0.49
1:A:141:ASP:O	1:A:141:ASP:OD2	2.30	0.49
2:A:301:CD8:OAG	2:A:301:CD8:OAH	2.30	0.49
1:D:168:GLU:O	1:D:169:LEU:O	2.30	0.49
1:D:122:LEU:HD22	1:D:134:ALA:HA	1.94	0.49
2:A:301:CD8:HACA	2:A:301:CD8:CAZ	2.34	0.49
1:B:293:ALA:C	1:D:283:GLU:OE1	2.56	0.49
1:D:233:ASP:OD2	1:D:246:ASP:OD1	2.30	0.49
1:B:70:SER:N	2:B:301:CD8:HACB	2.26	0.49
1:D:145:PRO:C	1:D:145(B):GLY:H	2.21	0.48
1:A:220:ARG:O	1:A:222:ARG:N	2.46	0.48
2:C:301:CD8:OAT	2:C:301:CD8:OAG	2.30	0.48
1:D:72:PHE:CD1	1:D:72:PHE:C	2.91	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
1:B:241:TYR:HB3	1:B:268:ALA:HA	1.96	0.48
1:C:97:TYR:N	1:C:97:TYR:CD2	2.82	0.48
2:C:301:CD8:CAO	2:C:301:CD8:HNAS	2.09	0.48
1:A:117:MET:HB2	1:A:122:LEU:HD21	1.95	0.48
1:B:70:SER:HA	2:B:301:CD8:CAC	2.42	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:D:153:ARG:HD3	1:D:157:ASP:O	2.13	0.47
1:A:251:TRP:NE1	1:A:258:PRO:HB3	2.30	0.47
2:A:301:CD8:OAH	2:A:301:CD8:CAZ	2.62	0.47
1:B:241:TYR:HA	1:B:271:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ILE:O	1:D:248:ALA:HB1	2.15	0.47
1:D:240:ASP:O	1:D:241:TYR:C	2.57	0.46
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:D:168:GLU:O	1:D:169:LEU:C	2.58	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:B:293:ALA:HB2	1:D:286:THR:CG2	2.46	0.46
1:C:237:THR:O	2:C:301:CD8:CAM	2.63	0.46
1:C:70:SER:HA	1:C:72:PHE:CE2	2.51	0.46
1:D:240:ASP:C	1:D:242:GLY:H	2.22	0.46
1:A:255:THR:O	1:A:255:THR:CG2	2.63	0.45
1:C:86:ASN:N	1:C:86:ASN:HD22	2.14	0.45
1:D:229:TRP:CE3	1:D:252:SER:HA	2.51	0.45
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:A:197:ASN:ND2	1:A:197:ASN:N	2.53	0.45
1:C:236:GLY:HA2	2:C:301:CD8:OAH	2.17	0.45
1:D:104:SER:OG	1:D:166:ALA:HB1	2.16	0.45
1:B:49:VAL:HB	1:B:58:ILE:HB	1.99	0.45
1:B:220:ARG:HD3	1:B:281:LEU:HD12	1.98	0.45
1:C:72:PHE:H	1:C:72:PHE:HD2	1.63	0.45
1:D:72:PHE:HE1	1:D:76:LEU:HD22	1.82	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:A:87:PRO:O	1:A:88:LEU:C	2.60	0.44
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.71	0.44
1:D:103:ARG:CB	1:D:167:PRO:HD3	2.48	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:144:GLY:C	1:D:145:PRO:O	2.60	0.43
1:C:72:PHE:O	1:C:75:PRO:CD	2.66	0.43
1:C:72:PHE:O	1:C:75:PRO:HD2	2.18	0.43
1:A:145(A):GLY:C	1:A:145(C):GLY:N	2.74	0.43
1:A:46:GLY:HA2	1:A:60:TYR:O	2.19	0.43
1:B:88:LEU:O	1:B:91:LEU:HG	2.18	0.43
1:D:229:TRP:CD2	1:D:252:SER:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ASP:O	1:D:242:GLY:N	2.52	0.43
1:D:37:LEU:O	1:D:41:TYR:HD1	2.01	0.43
1:C:129:TYR:O	1:C:130:SER:C	2.60	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:B:240:ASP:O	1:B:241:TYR:HB2	2.18	0.43
1:C:69:CYS:O	1:C:72:PHE:CD2	2.71	0.43
1:C:72:PHE:C	1:C:74:ALA:N	2.76	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:A:275:GLU:HA	1:A:276:PRO:HD3	1.91	0.42
1:D:178:ARG:O	1:D:179:ASP:HB2	2.19	0.42
1:A:220:ARG:O	1:A:223:ALA:N	2.45	0.42
1:C:76:LEU:HD12	1:C:76:LEU:O	2.18	0.42
1:D:143:GLY:O	1:D:145(C):GLY:HA2	2.18	0.42
1:A:117:MET:HA	1:A:121:GLN:NE2	2.34	0.42
1:D:70:SER:O	1:D:234:LYS:HE3	2.18	0.42
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: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: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: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:166:ALA:HA	1:D:167:PRO:HA	1.56	0.41
1:D:237:THR:HB	2:D:301:CD8:CAA	2.51	0.41
1:A:123:CYS:HB3	1:A:210:TRP:CZ3	2.55	0.41
1:B:94:LEU:HD12	1:B:94:LEU:HA	1.85	0.41
1:B:222:ARG:NH2	1:B:226:PRO:O	2.53	0.41
1:C:80:VAL:O	1:C:86:ASN:ND2	2.54	0.41
1:D:68:PHE:O	1:D:69:CYS:C	2.63	0.41
1:D:233:ASP:HB3	1:D:248:ALA:CB	2.48	0.41
1:A:263:VAL:HG12	1:A:281:LEU:CD2	2.41	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.57	0.41
1:D:115:THR:HG23	1:D:116:GLY:O	2.21	0.41
1:D:130:SER:HB3	2:D:301:CD8:CBE	2.51	0.41
1:A:140:ALA:C	1:A:142:LEU:N	2.64	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:D:172:ASP:O	1:D:241:TYR:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:PRO:HD3	1:D:241:TYR:CD2	2.57	0.41
1:A:166:ALA:HA	1:A:167:PRO:HA	1.54	0.40
2:C:301:CD8:CAO	2:C:301:CD8:CAM	2.93	0.40
1:B:220:ARG:NH1	1:B:237:THR:OG1	2.36	0.40
1:D:242:GLY:O	1:D:266:ASP:HA	2.21	0.40
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.51	0.40
1:C:72:PHE:O	1:C:73:LYS:C	2.64	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%)	6	19
1	B	252/285 (88%)	242 (96%)	9 (4%)	1 (0%)	30	57
1	C	252/285 (88%)	232 (92%)	17 (7%)	3 (1%)	10	30
1	D	263/285 (92%)	240 (91%)	19 (7%)	4 (2%)	8	25
All	All	1030/1140 (90%)	959 (93%)	58 (6%)	13 (1%)	9	28

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

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Mol	Chain	Res	Type
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%)	155 (93%)	11 (7%)	15	40
1	B	161/218 (74%)	149 (92%)	12 (8%)	12	34
1	C	161/218 (74%)	148 (92%)	13 (8%)	11	30
1	D	162/218 (74%)	154 (95%)	8 (5%)	22	52
All	All	650/872 (74%)	606 (93%)	44 (7%)	14	38

All (44) 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	255	THR
1	A	280	LEU
1	A	291	VAL
1	B	39	ARG
1	B	42	ASP
1	B	54	THR
1	B	68	PHE

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Mol	Chain	Res	Type
1	B	70	SER
1	B	88	LEU
1	B	96	THR
1	B	102	ILE
1	B	103	ARG
1	B	110	GLN
1	B	233	ASP
1	B	280	LEU
1	C	33	ARG
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	158	THR
1	C	255	THR
1	C	280	LEU
1	C	291	VAL
1	D	89	THR
1	D	130	SER
1	D	186	ILE
1	D	215	THR
1	D	232	ILE
1	D	247	ILE
1	D	267	ARG
1	D	280	LEU

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

Mol	Chain	Res	Type
1	A	112	HIS
1	A	121	GLN
1	A	197	ASN
1	A	245	ASN
1	B	90	HIS
1	B	121	GLN
1	B	184	HIS
1	B	245	ASN
1	C	86	ASN

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Mol	Chain	Res	Type
1	C	90	HIS
1	C	184	HIS
1	D	90	HIS
1	D	121	GLN

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](#)

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	$\# Z > 2$
3	PO4	D	302	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0
3	PO4	C	302	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0
2	CD8	D	301	1	22,25,25	2.95	6 (27%)	20,35,35	1.56	2 (10%)
3	PO4	B	302	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0
2	CD8	A	301	1	22,25,25	3.11	7 (31%)	20,35,35	2.18	7 (35%)
2	CD8	B	301	1	22,25,25	3.11	7 (31%)	20,35,35	2.11	4 (20%)
2	CD8	C	301	1	22,25,25	2.93	7 (31%)	20,35,35	1.62	4 (20%)

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	B	301	1	-	2/9/38/38	0/1/2/2
2	CD8	A	301	1	-	2/9/38/38	0/1/2/2
2	CD8	C	301	1	-	2/9/38/38	0/1/2/2
2	CD8	D	301	1	-	6/9/38/38	0/1/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CD8	CAO-CAX	-9.84	1.37	1.50
2	A	301	CD8	CAO-CAX	-9.68	1.37	1.50
2	C	301	CD8	CAO-CAX	-8.91	1.38	1.50
2	D	301	CD8	CAO-CAX	-8.17	1.39	1.50
2	D	301	CD8	CBB-NAQ	7.07	1.35	1.28
2	B	301	CD8	CBB-NAQ	6.02	1.34	1.28
2	A	301	CD8	CBB-CAY	-5.56	1.37	1.48
2	A	301	CD8	CBB-NAQ	5.49	1.33	1.28
2	C	301	CD8	CBB-CAY	-5.37	1.37	1.48
2	C	301	CD8	CBB-NAQ	5.36	1.33	1.28
2	B	301	CD8	CBB-CAY	-5.36	1.37	1.48
2	A	301	CD8	CBC-CAZ	-5.31	1.38	1.50
2	C	301	CD8	CBC-CAZ	-5.18	1.38	1.50
2	B	301	CD8	CBC-CAZ	-5.05	1.39	1.50
2	D	301	CD8	CBC-CAZ	-4.91	1.39	1.50
3	D	302	PO4	P-O1	4.69	1.61	1.50
3	C	302	PO4	P-O1	4.68	1.61	1.50
3	B	302	PO4	P-O1	4.66	1.61	1.50
2	D	301	CD8	CBB-CAY	-4.43	1.39	1.48
2	D	301	CD8	CAA-CAX	3.35	1.39	1.32
2	C	301	CD8	CAA-CAX	3.10	1.38	1.32
2	A	301	CD8	OAI-CAY	-2.91	1.22	1.30
2	B	301	CD8	CAA-CAX	2.90	1.38	1.32
2	B	301	CD8	OAI-CAY	-2.79	1.23	1.30
2	A	301	CD8	CAA-CAX	2.76	1.38	1.32
2	D	301	CD8	CBF-CBA	2.75	1.53	1.50
2	B	301	CD8	CBB-CAX	-2.40	1.38	1.46
2	C	301	CD8	CBB-CAX	-2.39	1.38	1.46
3	C	302	PO4	P-O3	2.38	1.61	1.54
2	A	301	CD8	CBB-CAX	-2.38	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	PO4	P-O3	2.36	1.61	1.54
3	B	302	PO4	P-O2	2.35	1.61	1.54
2	C	301	CD8	OAI-CAY	-2.34	1.24	1.30
3	D	302	PO4	P-O3	2.33	1.61	1.54
3	D	302	PO4	P-O2	2.32	1.61	1.54
3	C	302	PO4	P-O2	2.31	1.61	1.54
3	B	302	PO4	P-O4	-2.15	1.48	1.54
3	D	302	PO4	P-O4	-2.14	1.48	1.54
3	C	302	PO4	P-O4	-2.13	1.48	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CD8	CAC-OAT-CBF	-6.92	106.84	115.35
2	B	301	CD8	CAC-OAT-CBF	-6.29	107.62	115.35
2	D	301	CD8	CAC-OAT-CBF	-4.74	109.53	115.35
2	B	301	CD8	CAO-SAV-CBE	4.68	102.78	94.36
2	C	301	CD8	CBF-NAS-CAZ	-3.84	115.36	123.63
2	C	301	CD8	CAC-OAT-CBF	-3.37	111.22	115.35
2	A	301	CD8	CAO-SAV-CBE	3.23	100.18	94.36
2	A	301	CD8	CBF-NAS-CAZ	-3.09	116.96	123.63
2	C	301	CD8	CAO-SAV-CBE	3.09	99.92	94.36
2	D	301	CD8	CBF-NAS-CAZ	-3.08	116.98	123.63
2	A	301	CD8	OAH-CBA-CBF	-2.68	119.22	124.34
2	B	301	CD8	CAO-CAX-CAA	-2.56	116.80	121.59
2	A	301	CD8	CAO-CAX-CAA	-2.43	117.05	121.59
2	B	301	CD8	CBC-CAZ-NAS	-2.24	112.77	116.87
2	A	301	CD8	OAI-CAY-OAF	-2.08	118.95	123.90
2	C	301	CD8	OAH-CBA-CBF	-2.05	120.43	124.34
2	A	301	CD8	CBC-CAZ-NAS	-2.04	113.13	116.87

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	CD8	OAG-CAZ-CBC-CAN
2	D	301	CD8	OAG-CAZ-CBC-CAM
2	D	301	CD8	NAS-CAZ-CBC-CAN
2	D	301	CD8	NAS-CAZ-CBC-CAM
2	D	301	CD8	OAF-CAY-CBB-CAX
2	A	301	CD8	OAF-CAY-CBB-CAX
2	B	301	CD8	OAF-CAY-CBB-CAX

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Mol	Chain	Res	Type	Atoms
2	C	301	CD8	OAF-CAY-CBB-CAX
2	A	301	CD8	OAI-CAY-CBB-NAQ
2	B	301	CD8	OAI-CAY-CBB-NAQ
2	C	301	CD8	OAI-CAY-CBB-NAQ
2	D	301	CD8	OAI-CAY-CBB-NAQ

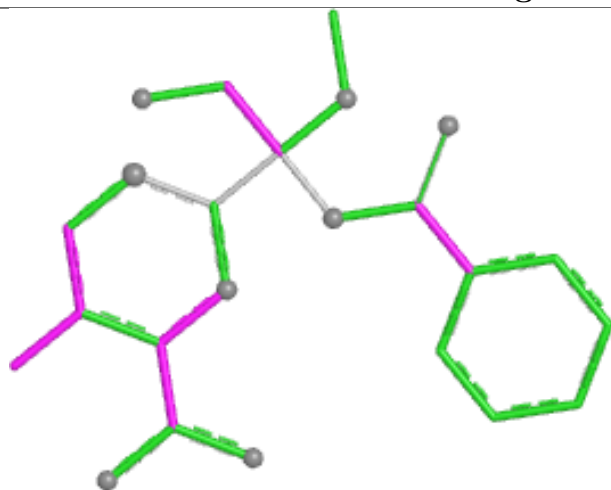
There are no ring outliers.

5 monomers are involved in 91 short contacts:

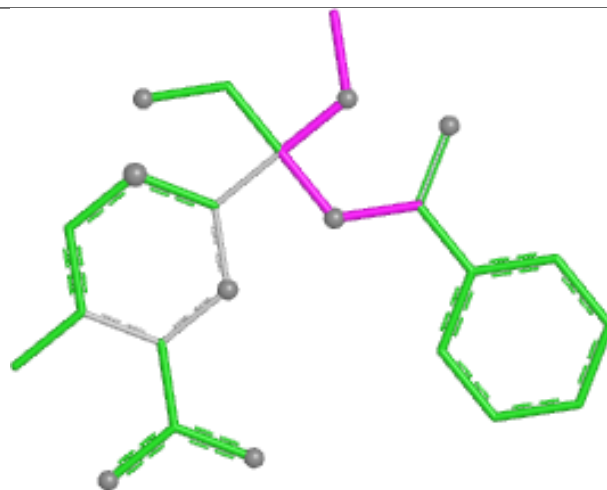
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	CD8	20	0
3	B	302	PO4	3	0
2	A	301	CD8	20	0
2	B	301	CD8	22	0
2	C	301	CD8	26	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

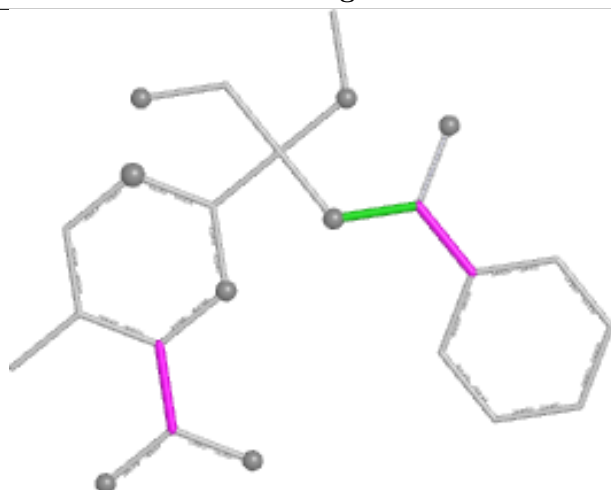
Ligand CD8 D 301



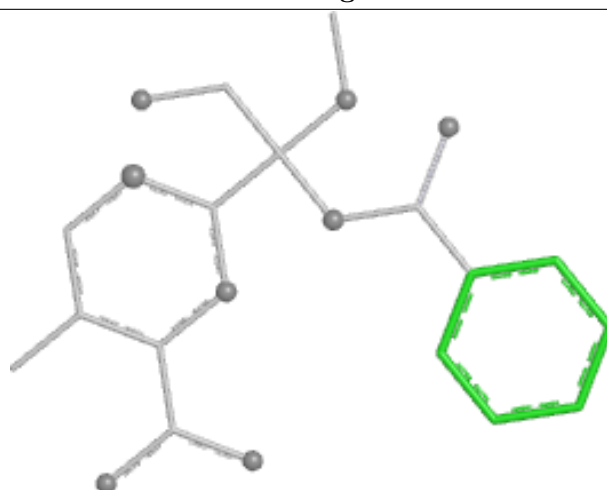
Bond lengths



Bond angles

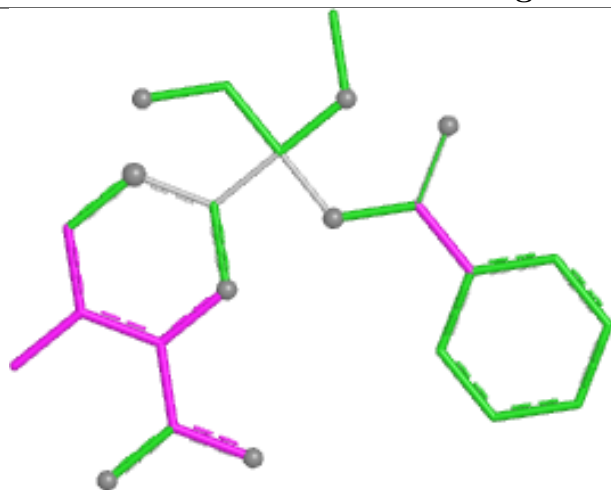


Torsions

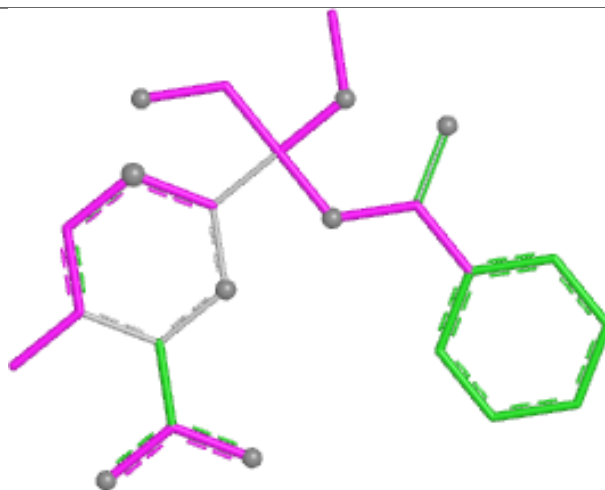


Rings

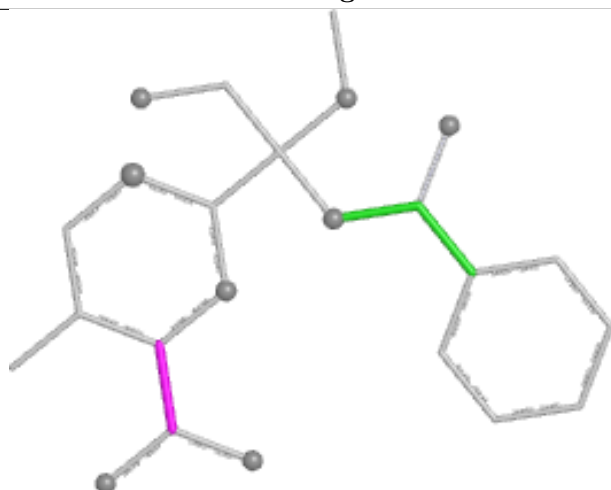
Ligand CD8 A 301



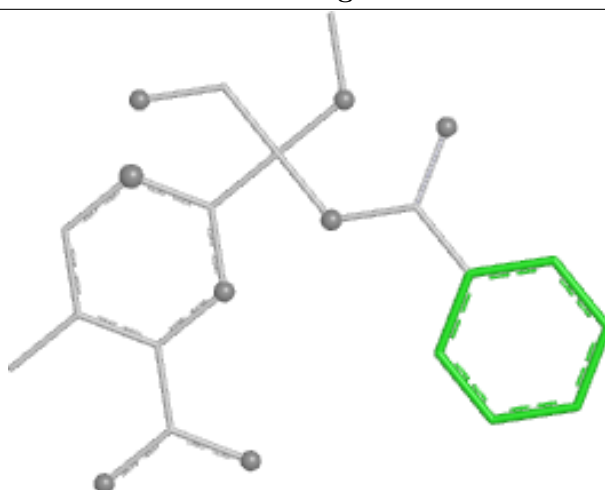
Bond lengths



Bond angles

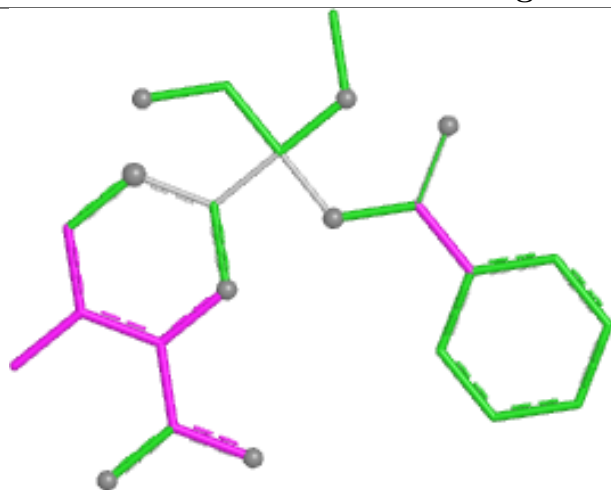


Torsions

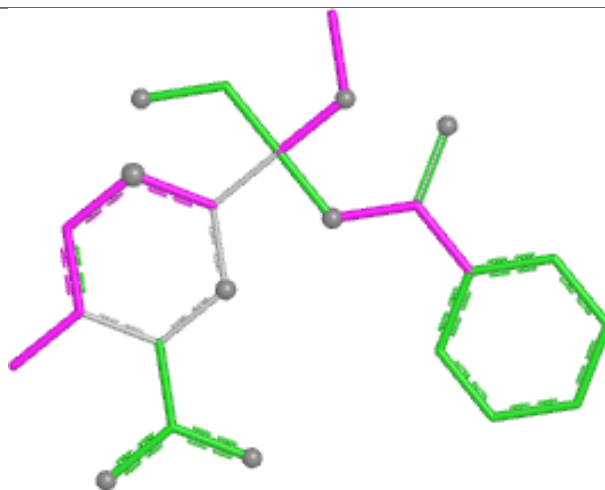


Rings

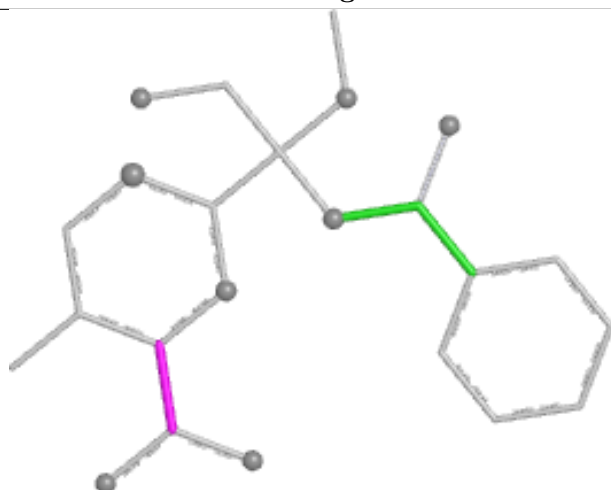
Ligand CD8 B 301



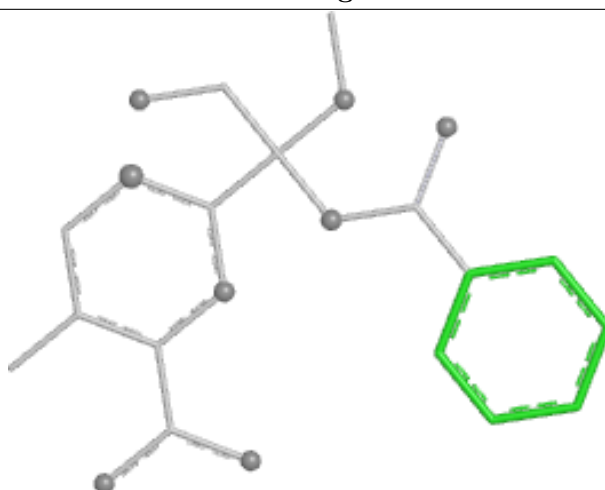
Bond lengths



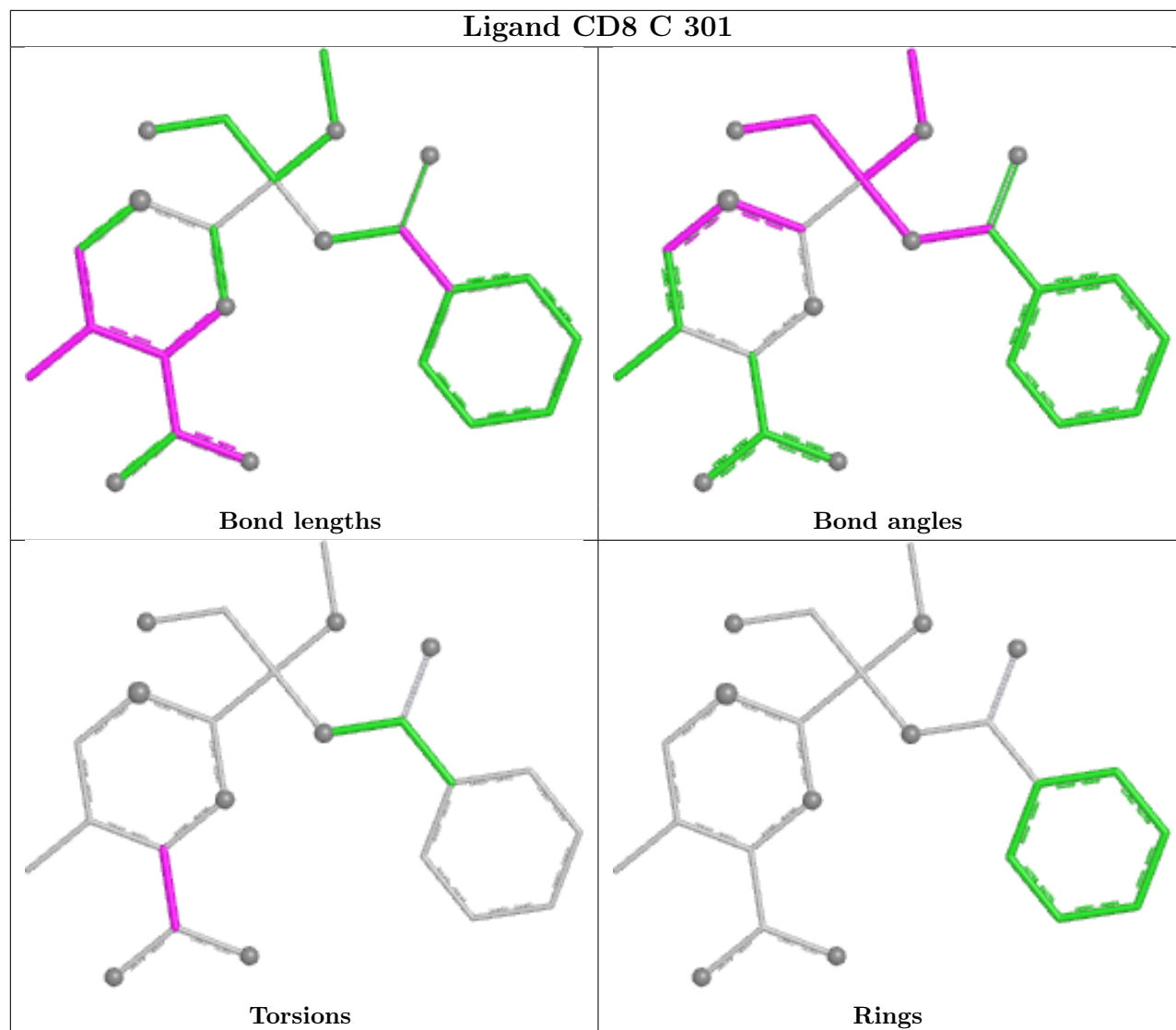
Bond angles



Torsions



Rings



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, 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	265/285 (92%)	1.28	52 (19%) 3 2	54, 71, 103, 125	0
1	B	256/285 (89%)	1.11	42 (16%) 4 4	53, 66, 92, 126	0
1	C	256/285 (89%)	1.17	47 (18%) 3 2	51, 69, 99, 121	0
1	D	265/285 (92%)	1.27	49 (18%) 3 2	56, 72, 107, 123	0
All	All	1042/1140 (91%)	1.21	190 (18%) 3 3	51, 69, 101, 126	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ASN	10.7
1	A	166	ALA	7.4
1	A	169	LEU	6.9
1	D	169	LEU	5.9
1	D	170	ASN	5.8
1	A	105	ILE	5.6
1	A	52	THR	5.5
1	A	115	THR	5.4
1	D	172	ASP	5.3
1	D	113	VAL	5.3
1	B	113	VAL	5.3
1	C	100	ASP	5.2
1	D	105	ILE	5.0
1	A	273	ASP	4.8
1	B	100	ASP	4.8
1	A	114	GLN	4.8
1	A	164	ALA	4.7
1	C	95	ILE	4.6
1	B	99	SER	4.6
1	C	177	GLU	4.6
1	B	158	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	171	ARG	4.5
1	A	113	VAL	4.5
1	A	275	GLU	4.4
1	D	168	GLU	4.4
1	A	95	ILE	4.4
1	B	103	ARG	4.3
1	A	99	SER	4.3
1	D	89	THR	4.3
1	C	293	ALA	4.2
1	B	282	ALA	4.2
1	D	142	LEU	4.1
1	C	92	ASP	4.1
1	B	162	LEU	4.1
1	B	176	ASP	4.1
1	D	29	ASP	4.1
1	D	42	ASP	4.1
1	D	228	ASP	4.0
1	D	164	ALA	4.0
1	C	173	PRO	4.0
1	D	158	THR	3.9
1	B	173	PRO	3.9
1	B	29	ASP	3.9
1	B	41	TYR	3.7
1	A	116	GLY	3.7
1	B	98	THR	3.7
1	A	53	GLY	3.6
1	C	228	ASP	3.6
1	C	247	ILE	3.6
1	D	171	ARG	3.6
1	B	163	ASP	3.5
1	A	255	THR	3.5
1	C	94	LEU	3.5
1	B	142	LEU	3.5
1	C	113	VAL	3.4
1	C	32	ASP	3.4
1	A	54	THR	3.4
1	C	111	GLN	3.4
1	C	110	GLN	3.4
1	C	174	PRO	3.3
1	C	175	GLY	3.3
1	D	202	ASP	3.3
1	A	72	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	209	ASP	3.3
1	D	166	ALA	3.3
1	D	111	GLN	3.3
1	C	212	ALA	3.2
1	A	228	ASP	3.2
1	D	116	GLY	3.2
1	B	202	ASP	3.1
1	D	107	PRO	3.1
1	A	110	GLN	3.1
1	C	255	THR	3.1
1	D	55	THR	3.1
1	B	277	ARG	3.1
1	D	86	ASN	3.1
1	D	102	ILE	3.1
1	A	42	ASP	3.0
1	A	168	GLU	3.0
1	D	167	PRO	3.0
1	D	95	ILE	3.0
1	A	271	GLY	3.0
1	C	83	GLN	2.9
1	A	172	ASP	2.9
1	C	89	THR	2.9
1	A	268	ALA	2.9
1	B	145	PRO	2.9
1	D	136	ASN	2.9
1	D	273	ASP	2.9
1	A	100	ASP	2.9
1	A	142	LEU	2.9
1	D	108	VAL	2.9
1	C	29	ASP	2.8
1	A	274	ALA	2.8
1	A	276	PRO	2.8
1	B	175	GLY	2.8
1	D	272	TYR	2.8
1	B	114	GLN	2.8
1	A	277	ARG	2.7
1	D	277	ARG	2.7
1	A	241	TYR	2.7
1	D	291	VAL	2.7
1	A	165	GLU	2.7
1	C	197	ASN	2.7
1	A	89	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	158	THR	2.7
1	D	140	ALA	2.6
1	A	256	GLY	2.6
1	C	176	ASP	2.6
1	A	270	GLY	2.6
1	D	156	GLY	2.6
1	B	67	ALA	2.6
1	B	157	ASP	2.6
1	C	105	ILE	2.6
1	C	88	LEU	2.6
1	B	185	ALA	2.6
1	B	160	SER	2.5
1	A	157	ASP	2.5
1	D	100	ASP	2.5
1	B	111	GLN	2.5
1	C	96	THR	2.5
1	A	162	LEU	2.5
1	D	218	ALA	2.5
1	D	99	SER	2.5
1	A	55	THR	2.5
1	B	52	THR	2.5
1	B	115	THR	2.5
1	D	88	LEU	2.5
1	D	53	GLY	2.5
1	B	56	ALA	2.5
1	C	216	THR	2.4
1	D	174	PRO	2.4
1	B	161	ARG	2.4
1	C	71	THR	2.4
1	C	256	GLY	2.4
1	D	90	HIS	2.4
1	D	123	CYS	2.4
1	D	79	ALA	2.4
1	B	177	GLU	2.4
1	C	210	TRP	2.4
1	D	269	GLY	2.4
1	A	163	ASP	2.3
1	A	111	GLN	2.3
1	D	41	TYR	2.3
1	D	104	SER	2.3
1	C	161	ARG	2.3
1	C	236	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	122	LEU	2.3
1	B	149	THR	2.3
1	B	197	ASN	2.3
1	C	46	GLY	2.3
1	D	157	ASP	2.3
1	C	114	GLN	2.3
1	C	242	GLY	2.2
1	C	290	GLY	2.2
1	B	97	TYR	2.2
1	D	241	TYR	2.2
1	B	269	GLY	2.2
1	B	137	LEU	2.2
1	C	81	LEU	2.2
1	C	69	CYS	2.2
1	A	174	PRO	2.2
1	C	91	LEU	2.2
1	C	116	GLY	2.2
1	C	281	LEU	2.2
1	A	103	ARG	2.2
1	B	273	ASP	2.2
1	A	80	VAL	2.2
1	C	272	TYR	2.1
1	B	144	GLY	2.1
1	A	102	ILE	2.1
1	A	149	THR	2.1
1	D	255	THR	2.1
1	C	59	GLU	2.1
1	C	108	VAL	2.1
1	B	32	ASP	2.1
1	B	278	GLU	2.1
1	D	96	THR	2.1
1	C	179	ASP	2.0
1	B	218	ALA	2.0
1	D	70	SER	2.0
1	A	94	LEU	2.0
1	A	236	GLY	2.0
1	B	156	GLY	2.0
1	A	151	TYR	2.0
1	A	202	ASP	2.0
1	B	293	ALA	2.0
1	C	42	ASP	2.0
1	A	83	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	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](#)

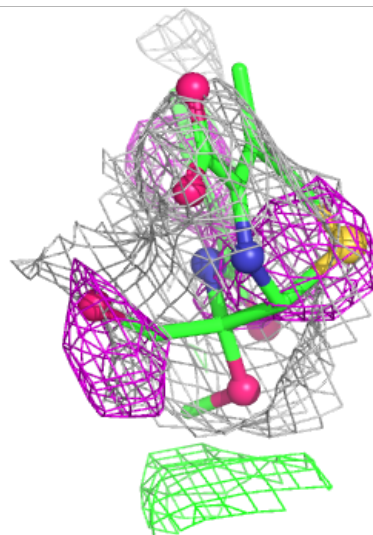
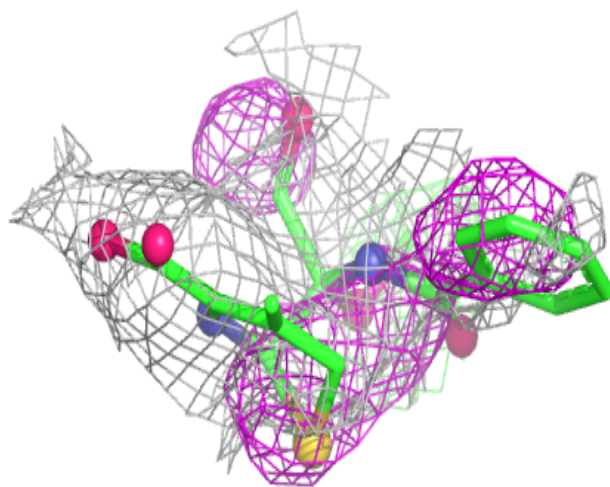
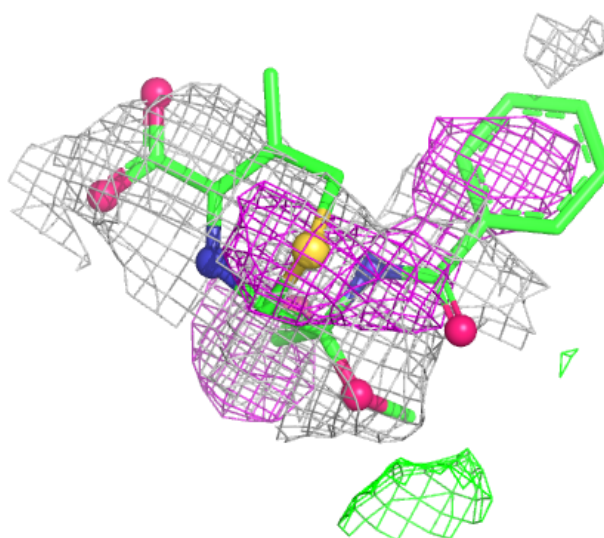
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CD8	C	301	24/24	0.51	0.23	93,102,110,115	0
2	CD8	B	301	24/24	0.66	0.24	88,95,108,109	0
3	PO4	D	302	5/5	0.71	0.17	92,104,116,120	0
3	PO4	C	302	5/5	0.73	0.12	96,100,115,120	0
2	CD8	D	301	24/24	0.74	0.17	76,86,98,102	0
2	CD8	A	301	24/24	0.77	0.17	77,87,94,100	0
3	PO4	B	302	5/5	0.86	0.14	85,90,95,102	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

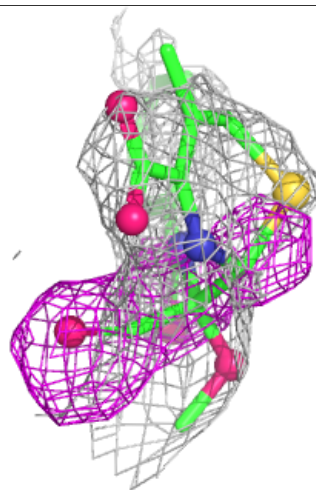
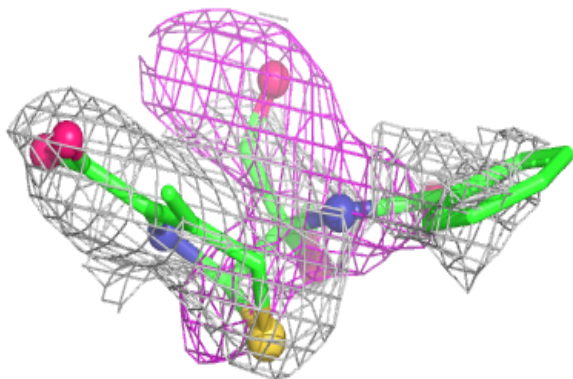
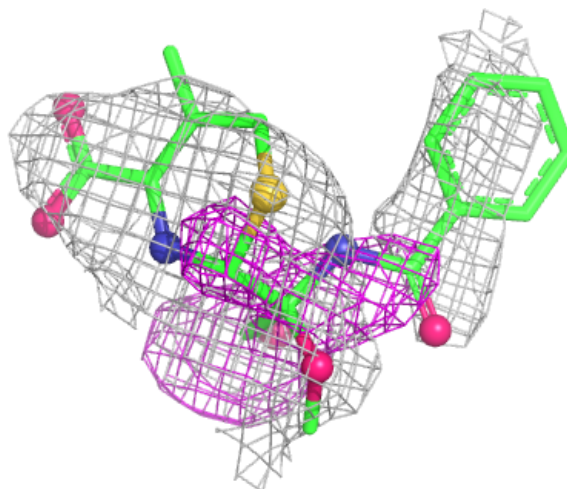
Electron density around CD8 C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



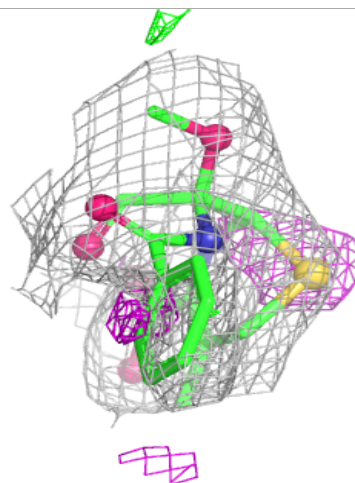
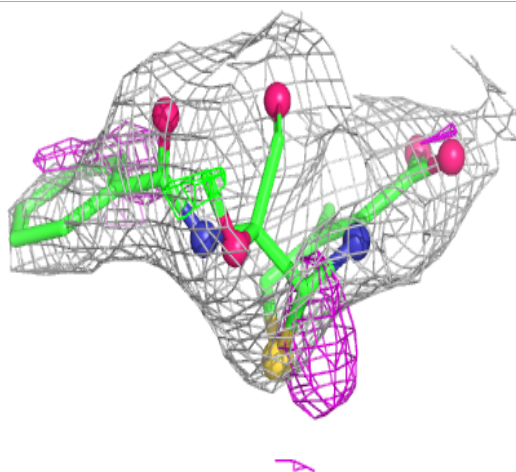
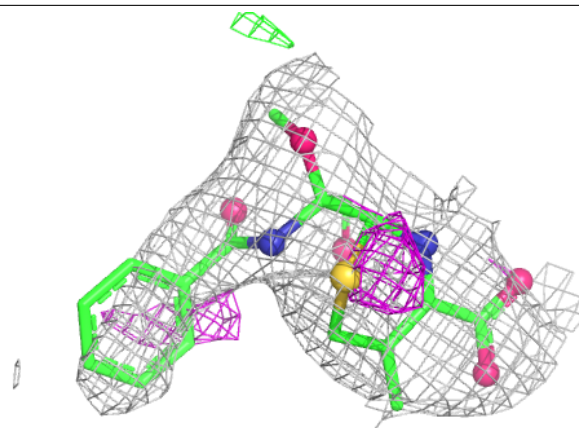
Electron density around CD8 B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



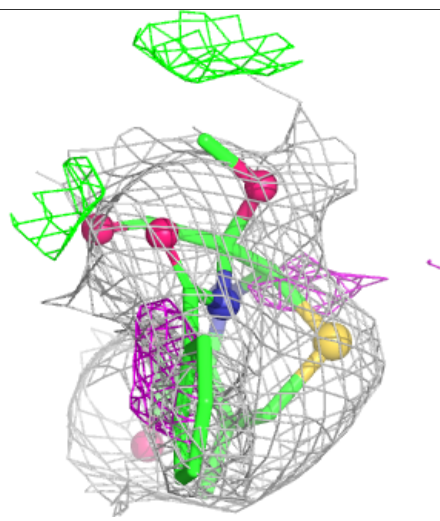
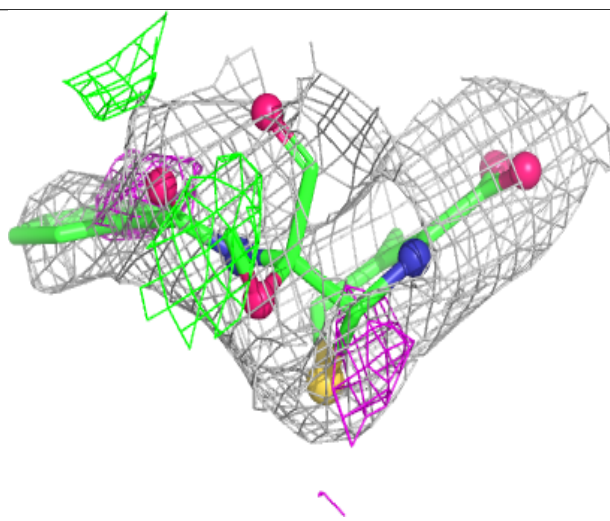
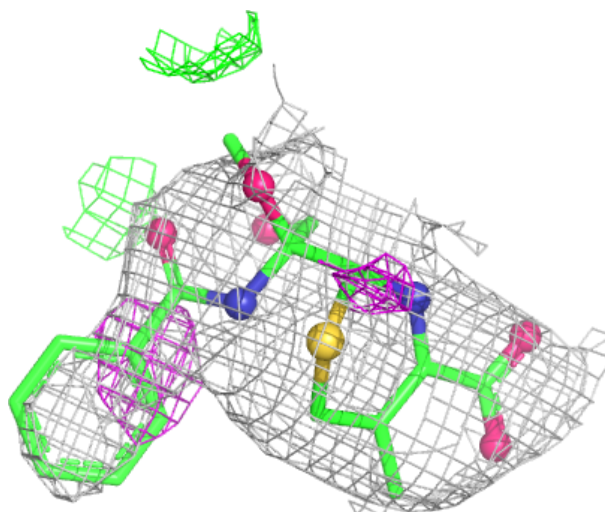
Electron density around CD8 D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CD8 A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.