



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:07 PM UTC

PDB ID : 3VFH / pdb_00003vfh
Title : BlaC E166A CDC-1 Acyl-Intermediate
Authors : Mire, J.A.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2012-01-09
Resolution : 2.57 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

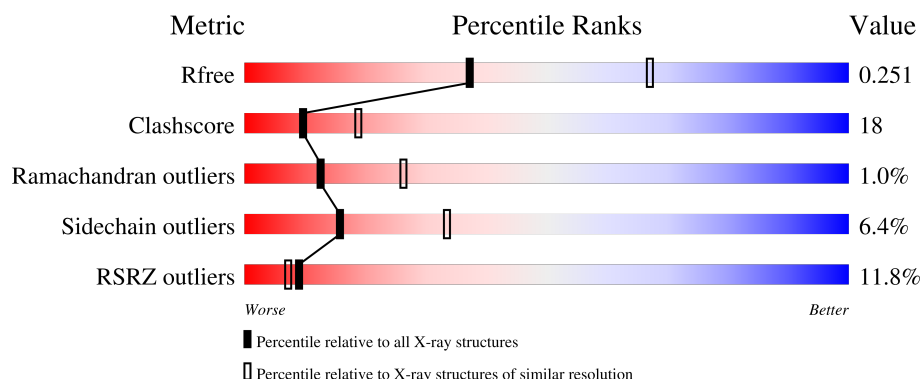
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	10% 71% 20% • 7%
1	B	285	11% 69% 20% • 7%
1	C	285	11% 65% 24% • 7%
1	D	285	11% 63% 29% • 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	PO4	A	301	-	X	-	-
2	PO4	A	302	-	X	-	-
2	PO4	A	303	-	X	-	-
2	PO4	B	302	-	X	-	-
2	PO4	C	302	-	X	-	-
2	PO4	D	301	-	X	X	-
2	PO4	D	302	-	X	-	-
3	CD6	B	301	-	-	X	-
3	CD6	C	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8123 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
			1984	1241	352	385	6			
1	B	265	Total	C	N	O	S	0	0	0
			1984	1241	352	385	6			
1	C	265	Total	C	N	O	S	0	0	0
			1980	1239	352	383	6			
1	D	265	Total	C	N	O	S	0	0	0
			1980	1239	351	384	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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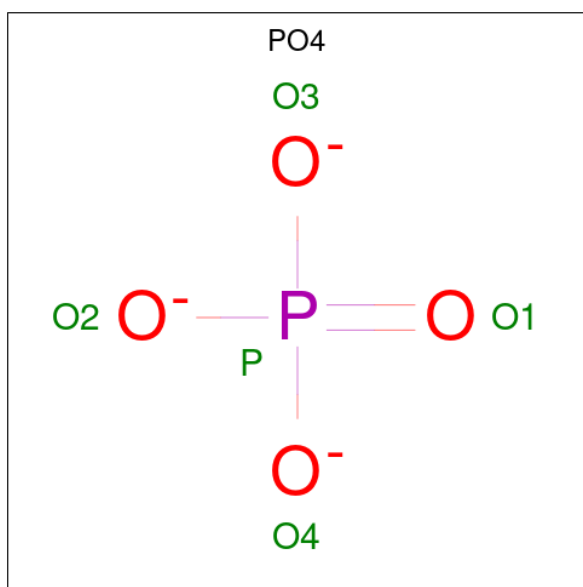
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP P0C5C1
B	10	GLY	-	expression tag	UNP P0C5C1
B	11	SER	-	expression tag	UNP P0C5C1
B	12	SER	-	expression tag	UNP P0C5C1
B	13	HIS	-	expression tag	UNP P0C5C1
B	14	HIS	-	expression tag	UNP P0C5C1
B	15	HIS	-	expression tag	UNP P0C5C1
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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



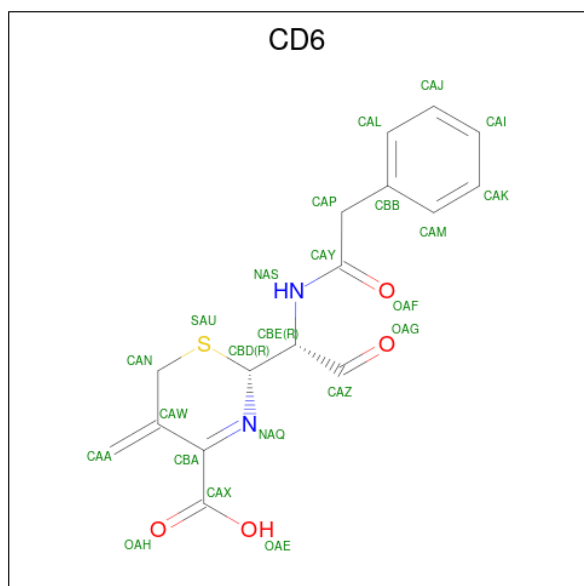
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is (2R)-5-methylidene-2-[(1R)-2-oxo-1-[(phenylacetyl)amino]ethyl]-5,6-dihydro-2H-1,3-thiazine-4-carboxylic acid (CCD ID: CD6) (formula: C₁₆H₁₆N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			23	16	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			23	16	2	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		

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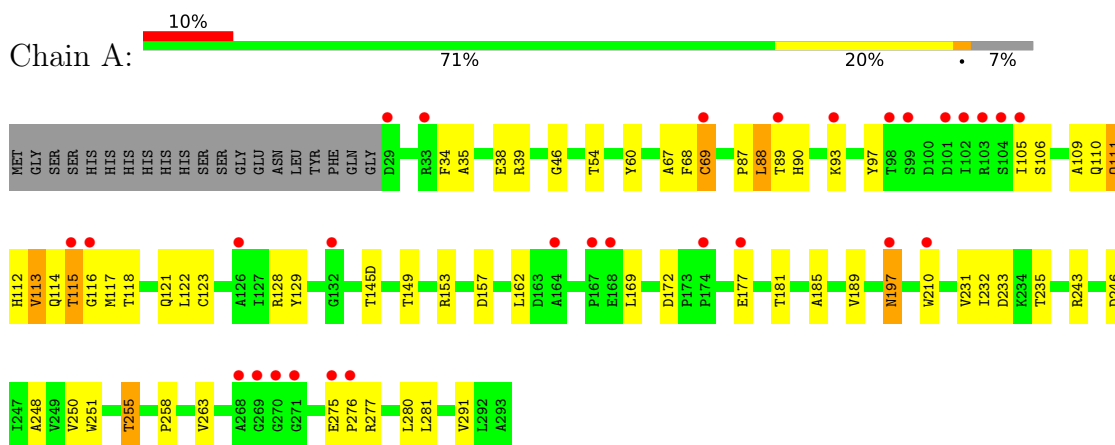
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	28	Total 28	O 28	0	0
4	C	32	Total 32	O 32	0	0
4	D	22	Total 22	O 22	0	0

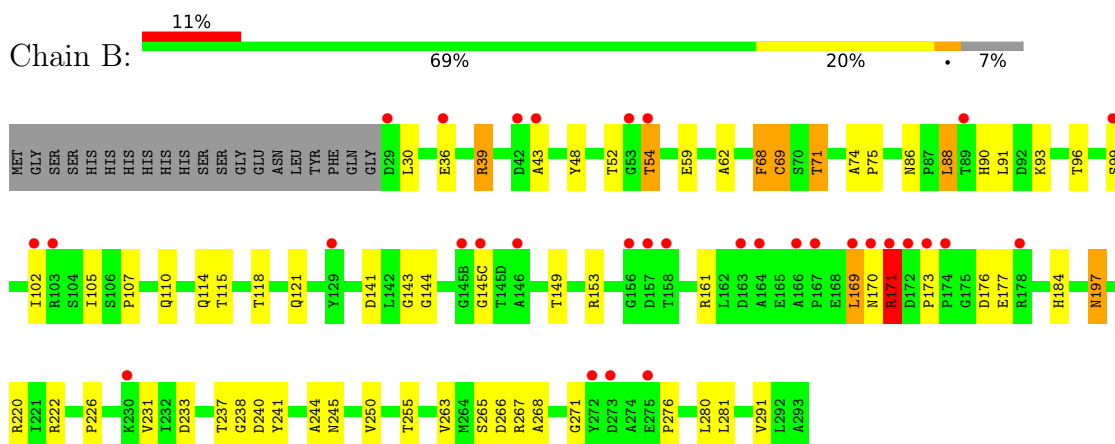
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

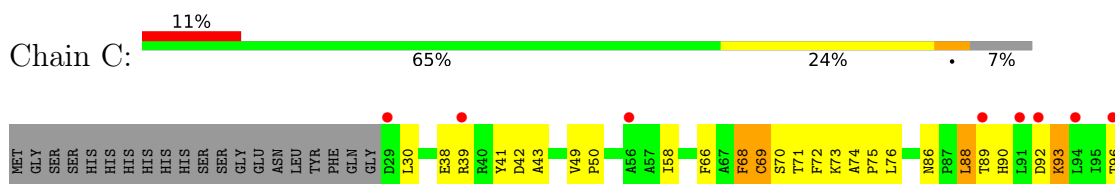
- Molecule 1: Beta-lactamase

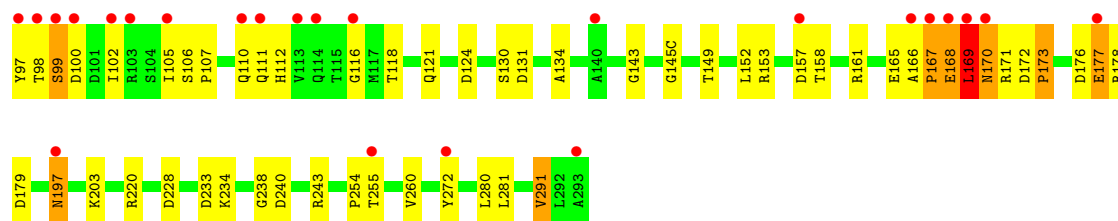


- Molecule 1: Beta-lactamase

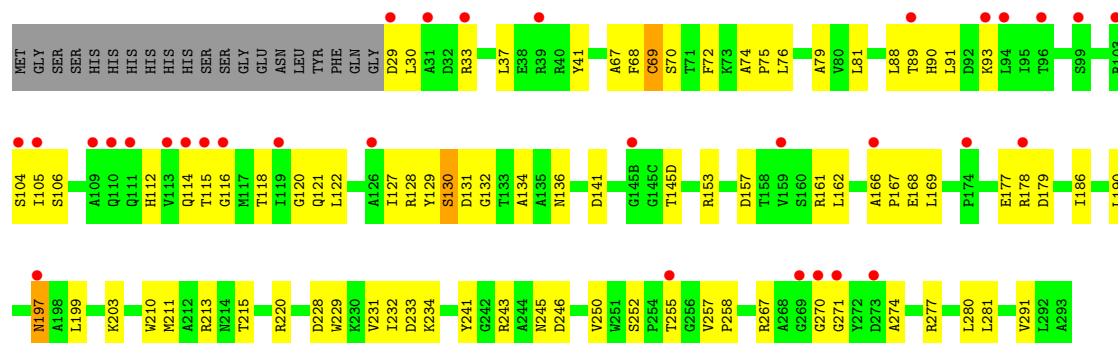


- Molecule 1: Beta-lactamase





• Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.40Å 97.46Å 110.96Å 90.00° 108.37° 90.00°	Depositor
Resolution (Å)	47.09 – 2.57 47.09 – 2.57	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.09-2.57) 97.4 (47.09-2.57)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.225 , 0.252 0.225 , 0.251	Depositor DCC
R_{free} test set	2529 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8123	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: PO4, CD6

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	0.55	0/2023	0.84	0/2762
1	B	0.57	0/2023	0.93	2/2762 (0.1%)
1	C	0.59	0/2019	0.88	2/2757 (0.1%)
1	D	0.59	0/2019	0.92	5/2757 (0.2%)
All	All	0.57	0/8084	0.90	9/11038 (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	7.71	125.21	119.66
1	D	199	LEU	C-N-CA	7.71	125.21	119.66
1	B	144	GLY	CA-C-N	6.41	126.38	119.78
1	B	144	GLY	C-N-CA	6.41	126.38	119.78
1	D	233	ASP	N-CA-C	6.30	117.80	108.60
1	C	66	PHE	N-CA-C	-5.93	100.28	109.24
1	C	233	ASP	N-CA-C	5.75	117.00	108.60
1	D	106	SER	CA-C-N	5.06	124.78	119.82
1	D	106	SER	C-N-CA	5.06	124.78	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	1984	0	1955	57	0
1	B	1984	0	1954	71	0
1	C	1980	0	1950	86	0
1	D	1980	0	1949	72	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	10	0	0	2	0
3	B	23	0	14	15	0
3	C	23	0	14	10	0
4	A	32	0	0	1	0
4	B	28	0	0	1	0
4	C	32	0	0	2	0
4	D	22	0	0	2	0
All	All	8123	0	7836	281	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 18.

All (281) 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:169:LEU:HD12	1:C:170:ASN:N	1.36	1.41
1:B:169:LEU:HD12	1:B:169:LEU:O	1.37	1.25
1:B:171:ARG:CB	1:B:171:ARG:HH11	1.48	1.25
1:B:171:ARG:NH1	1:B:171:ARG:HB2	1.56	1.18
1:B:43:ALA:HB2	1:B:267:ARG:HG2	1.27	1.15
1:B:39:ARG:HH21	1:B:39:ARG:HB3	1.10	1.07
1:B:171:ARG:HH11	1:B:171:ARG:HB2	0.92	1.05
3:C:301:CD6:HAAA	3:C:301:CD6:OAE	1.55	1.03
3:B:301:CD6:OAE	3:B:301:CD6:HAAA	1.55	1.00
1:B:169:LEU:HD12	1:B:169:LEU:C	1.84	0.99
1:B:171:ARG:HH11	1:B:171:ARG:CG	1.78	0.94
1:B:39:ARG:HH21	1:B:39:ARG:CB	1.81	0.94
1:C:169:LEU:CD1	1:C:170:ASN:N	2.31	0.92
1:A:197:ASN:HD22	1:A:197:ASN:H	1.14	0.89
1:C:169:LEU:HD12	1:C:169:LEU:C	1.98	0.88
3:C:301:CD6:HAN	3:C:301:CD6:NAS	1.90	0.87
1:D:112:HIS:HD2	1:D:115:THR:HG21	1.39	0.87
1:B:39:ARG:HB3	1:B:39:ARG:NH2	1.92	0.84
1:C:86:ASN:CG	1:C:90:HIS:ND1	2.36	0.83
3:B:301:CD6:HAN	3:B:301:CD6:NAS	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ALA:CB	1:B:267:ARG:HG2	2.08	0.83
1:A:111:GLN:NE2	3:B:301:CD6:CAI	2.42	0.82
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	0.81
1:D:197:ASN:HD22	1:D:197:ASN:H	1.27	0.79
1:C:169:LEU:HD12	1:C:170:ASN:CA	2.12	0.79
1:C:170:ASN:HD22	1:C:171:ARG:N	1.80	0.79
1:A:114:GLN:NE2	1:B:171:ARG:HE	1.81	0.78
1:D:197:ASN:H	1:D:197:ASN:ND2	1.80	0.78
1:A:114:GLN:HE22	1:B:171:ARG:HE	1.27	0.78
1:B:36:GLU:HG3	1:B:39:ARG:HH22	1.49	0.77
1:C:169:LEU:HD12	1:C:170:ASN:H	1.44	0.77
3:C:301:CD6:OAE	3:C:301:CD6:CAA	2.30	0.77
1:A:111:GLN:HE21	3:B:301:CD6:CAK	1.98	0.76
1:D:255:THR:HG22	1:D:255:THR:O	1.86	0.75
1:A:112:HIS:HB3	1:A:115:THR:HG23	1.69	0.74
1:B:68:PHE:O	1:B:69:CYS:HB2	1.88	0.73
1:A:197:ASN:H	1:A:197:ASN:ND2	1.86	0.71
1:B:237:THR:O	3:B:301:CD6:HAPA	1.90	0.71
1:C:171:ARG:O	1:C:171:ARG:HG3	1.88	0.71
1:C:228:ASP:OD1	1:C:254:PRO:HG3	1.91	0.71
3:C:301:CD6:HAN	3:C:301:CD6:CAY	2.20	0.70
1:B:171:ARG:NH1	1:B:171:ARG:CG	2.46	0.69
1:C:170:ASN:HD22	1:C:171:ARG:H	1.38	0.69
1:B:197:ASN:HD22	1:B:197:ASN:H	1.39	0.69
1:D:231:VAL:HG22	1:D:250:VAL:HG12	1.75	0.69
1:B:263:VAL:CG1	1:B:281:LEU:HD22	2.23	0.69
1:D:112:HIS:HD2	1:D:115:THR:CG2	2.07	0.68
1:C:255:THR:O	1:C:255:THR:HG22	1.93	0.68
1:C:168:GLU:O	1:C:171:ARG:N	2.20	0.68
1:C:171:ARG:NH2	1:D:114:GLN:HE22	1.91	0.68
1:A:145(D):THR:HB	1:A:162:LEU:O	1.94	0.67
1:D:112:HIS:CD2	1:D:115:THR:HG21	2.26	0.67
1:A:67:ALA:HB3	1:A:243:ARG:HD3	1.75	0.67
1:B:220:ARG:NH1	1:B:237:THR:OG1	2.20	0.67
1:B:43:ALA:HB2	1:B:267:ARG:CG	2.17	0.66
1:B:169:LEU:O	1:B:169:LEU:CD1	2.30	0.66
1:B:220:ARG:NH2	1:B:245:ASN:O	2.27	0.66
1:C:97:TYR:CE2	1:C:116:GLY:HA2	2.29	0.66
1:C:169:LEU:CD1	1:C:169:LEU:C	2.65	0.66
1:C:68:PHE:O	1:C:69:CYS:HB2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLU:O	1:C:170:ASN:N	2.29	0.66
1:A:111:GLN:HE21	3:B:301:CD6:CAI	2.07	0.66
1:A:69:CYS:O	1:A:169:LEU:HD11	1.96	0.65
1:B:169:LEU:C	1:B:169:LEU:CD1	2.60	0.65
1:D:90:HIS:HD2	1:D:93:LYS:NZ	1.94	0.64
1:A:112:HIS:O	1:A:116:GLY:N	2.28	0.63
1:B:118:THR:H	1:B:121:GLN:NE2	1.96	0.63
1:B:171:ARG:CB	1:B:171:ARG:NH1	2.30	0.63
1:B:231:VAL:HG22	1:B:250:VAL:HG12	1.81	0.62
1:D:220:ARG:HD3	1:D:281:LEU:HD12	1.80	0.62
1:A:111:GLN:NE2	3:B:301:CD6:CAK	2.61	0.62
1:C:220:ARG:HD3	1:C:281:LEU:HD12	1.80	0.62
3:C:301:CD6:NAS	3:C:301:CD6:CAN	2.61	0.62
1:C:149:THR:O	1:C:153:ARG:HG2	1.99	0.62
1:B:43:ALA:HB1	1:B:266:ASP:O	2.00	0.62
1:D:128:ARG:HD2	1:D:213:ARG:O	1.99	0.62
1:B:220:ARG:HD3	1:B:281:LEU:HD12	1.82	0.61
1:C:172:ASP:O	1:C:173:PRO:O	2.19	0.60
1:B:237:THR:O	3:B:301:CD6:CAP	2.49	0.60
3:B:301:CD6:HAN	3:B:301:CD6:CAY	2.32	0.60
1:B:48:TYR:CE2	1:B:184:HIS:HD2	2.21	0.59
1:C:99:SER:CB	1:D:105:ILE:HG12	2.32	0.59
1:C:168:GLU:O	1:C:169:LEU:C	2.45	0.59
1:C:111:GLN:NE2	2:D:301:PO4:O1	2.35	0.59
1:A:68:PHE:O	1:A:69:CYS:HB2	2.02	0.59
1:D:130:SER:OG	2:D:301:PO4:O3	2.20	0.59
1:D:131:ASP:HB3	1:D:134:ALA:HB3	1.83	0.59
1:D:145(D):THR:HB	1:D:162:LEU:O	2.02	0.59
1:D:168:GLU:H	1:D:168:GLU:CD	2.11	0.58
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.34	0.58
3:B:301:CD6:NAS	3:B:301:CD6:CAN	2.64	0.58
1:C:97:TYR:OH	1:C:112:HIS:HB2	2.04	0.58
1:D:197:ASN:HD22	1:D:197:ASN:N	1.94	0.58
1:B:220:ARG:HH12	1:B:237:THR:HG1	1.47	0.57
1:D:76:LEU:O	1:D:76:LEU:HD12	2.04	0.57
1:A:110:GLN:O	1:A:110:GLN:HG3	2.02	0.57
1:C:124:ASP:OD2	2:C:302:PO4:O1	2.22	0.57
1:C:167:PRO:O	1:C:169:LEU:N	2.38	0.57
1:C:99:SER:CB	1:D:105:ILE:CG1	2.82	0.57
1:C:49:VAL:HB	1:C:58:ILE:HB	1.86	0.57
1:A:149:THR:O	1:A:153:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TYR:CZ	1:B:184:HIS:CD2	2.94	0.56
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.67	0.56
1:D:68:PHE:O	1:D:69:CYS:HB2	2.06	0.56
1:A:118:THR:O	1:A:122:LEU:HG	2.07	0.55
1:B:90:HIS:HE1	1:B:141:ASP:OD2	1.89	0.55
1:D:112:HIS:CD2	1:D:115:THR:CG2	2.87	0.55
1:D:220:ARG:NH2	1:D:245:ASN:O	2.37	0.55
1:A:185:ALA:O	1:A:189:VAL:HG23	2.06	0.55
1:A:34:PHE:O	1:A:38:GLU:HG3	2.06	0.55
1:D:90:HIS:CD2	1:D:93:LYS:NZ	2.75	0.55
1:C:167:PRO:O	1:C:168:GLU:C	2.50	0.54
1:A:232:ILE:O	1:A:248:ALA:HB1	2.07	0.54
1:B:197:ASN:HD22	1:B:197:ASN:N	2.00	0.54
1:B:118:THR:H	1:B:121:GLN:HE21	1.55	0.54
1:A:35:ALA:O	1:A:39:ARG:HG3	2.08	0.54
1:B:171:ARG:NH1	1:B:171:ARG:HG3	2.20	0.54
1:D:29:ASP:N	4:D:415:HOH:O	2.41	0.53
1:A:250:VAL:O	1:A:258:PRO:HA	2.07	0.53
1:B:39:ARG:HH21	1:B:39:ARG:CG	2.21	0.53
1:D:190:LEU:HD11	1:D:211:MET:HE1	1.91	0.53
1:C:99:SER:OG	1:D:105:ILE:CG1	2.57	0.53
1:C:240:ASP:HB3	1:C:272:TYR:O	2.08	0.53
1:C:30:LEU:HD22	1:C:291:VAL:HG21	1.90	0.53
1:C:152:LEU:O	1:C:157:ASP:HB3	2.08	0.53
1:C:98:THR:O	1:C:100:ASP:N	2.42	0.53
1:C:110:GLN:NE2	1:D:129:TYR:O	2.41	0.53
1:C:124:ASP:C	1:C:124:ASP:OD1	2.51	0.53
1:D:104:SER:OG	1:D:132:GLY:HA3	2.09	0.53
1:D:69:CYS:O	1:D:72:PHE:HD2	1.92	0.53
1:D:167:PRO:HD2	1:D:168:GLU:OE1	2.08	0.53
1:D:255:THR:O	1:D:255:THR:CG2	2.54	0.53
1:C:105:ILE:HG22	1:C:107:PRO:HD3	1.91	0.52
1:A:197:ASN:HD22	1:A:197:ASN:N	1.86	0.52
1:C:99:SER:HB2	1:D:105:ILE:CG1	2.40	0.52
1:A:231:VAL:HG22	1:A:250:VAL:HG12	1.91	0.52
1:C:38:GLU:HG2	1:C:43:ALA:O	2.10	0.52
1:C:172:ASP:O	1:C:173:PRO:C	2.53	0.51
1:D:30:LEU:HD22	1:D:291:VAL:HG21	1.92	0.51
1:A:90:HIS:HD2	1:A:93:LYS:NZ	2.08	0.51
3:B:301:CD6:HAN	3:B:301:CD6:HNAS	1.73	0.51
1:A:118:THR:H	1:A:121:GLN:NE2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ARG:HD3	1:D:177:GLU:O	2.11	0.50
1:C:165:GLU:O	1:C:166:ALA:C	2.54	0.50
1:D:118:THR:H	1:D:121:GLN:NE2	2.09	0.50
1:C:238:GLY:HA2	3:C:301:CD6:HAPA	1.93	0.50
1:C:73:LYS:HB2	1:C:234:LYS:HE3	1.93	0.49
1:D:136:ASN:HD21	1:D:166:ALA:HB3	1.77	0.49
1:C:58:ILE:HD11	1:C:291:VAL:HG11	1.95	0.49
1:A:129:TYR:O	1:B:110:GLN:NE2	2.41	0.49
1:B:149:THR:O	1:B:153:ARG:HG2	2.13	0.49
1:B:68:PHE:O	1:B:71:THR:OG1	2.30	0.49
1:C:68:PHE:O	1:C:71:THR:OG1	2.30	0.49
1:B:244:ALA:HB2	1:B:276:PRO:HB3	1.95	0.48
1:C:86:ASN:CB	1:C:90:HIS:ND1	2.76	0.48
1:C:131:ASP:OD1	1:C:134:ALA:N	2.40	0.48
1:C:167:PRO:O	1:C:169:LEU:HG	2.13	0.48
1:C:68:PHE:HB2	1:C:179:ASP:O	2.12	0.48
1:A:105:ILE:CG1	1:B:99:SER:OG	2.61	0.48
1:C:99:SER:OG	1:D:105:ILE:N	2.46	0.48
1:A:233:ASP:HB3	1:A:248:ALA:HB2	1.94	0.48
1:D:122:LEU:HD22	1:D:134:ALA:HA	1.94	0.48
1:C:50:PRO:HD2	1:C:260:VAL:O	2.14	0.48
1:C:97:TYR:HE2	1:C:116:GLY:HA2	1.76	0.48
1:C:99:SER:OG	1:D:105:ILE:HG13	2.14	0.48
1:D:153:ARG:HD3	1:D:157:ASP:O	2.13	0.48
1:C:130:SER:OG	3:C:301:CD6:NAQ	2.44	0.48
1:D:168:GLU:OE1	1:D:168:GLU:N	2.30	0.48
1:B:52:THR:OG1	1:B:54:THR:HG23	2.14	0.47
1:C:99:SER:CB	1:D:105:ILE:HG13	2.43	0.47
1:C:170:ASN:ND2	1:C:171:ARG:N	2.56	0.47
1:B:161:ARG:HH21	1:B:177:GLU:HB3	1.79	0.47
1:B:143:GLY:O	1:B:145(C):GLY:HA2	2.14	0.47
1:B:241:TYR:HB3	1:B:268:ALA:HA	1.96	0.47
1:C:58:ILE:HD11	1:C:291:VAL:CG1	2.45	0.47
1:A:117:MET:HB2	1:A:122:LEU:HD21	1.95	0.47
1:C:99:SER:HB2	1:D:105:ILE:HG13	1.95	0.47
1:C:118:THR:H	1:C:121:GLN:NE2	2.13	0.47
1:D:91:LEU:HD22	1:D:120:GLY:HA2	1.96	0.47
1:B:237:THR:HB	3:B:301:CD6:CAA	2.44	0.47
1:B:241:TYR:HA	1:B:271:GLY:O	2.15	0.47
1:A:251:TRP:NE1	1:A:258:PRO:HB3	2.30	0.47
1:A:90:HIS:HD2	1:A:93:LYS:HZ1	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:CYS:O	1:C:72:PHE:HD2	1.98	0.46
1:D:90:HIS:HD2	1:D:93:LYS:HZ1	1.61	0.46
1:D:229:TRP:CE3	1:D:252:SER:HA	2.51	0.46
1:A:105:ILE:HG13	1:B:99:SER:OG	2.16	0.46
1:C:41:TYR:O	1:C:42:ASP:HB2	2.15	0.46
1:C:168:GLU:O	1:C:170:ASN:ND2	2.48	0.46
1:A:263:VAL:CG1	1:A:281:LEU:HD22	2.40	0.46
1:D:90:HIS:HD2	1:D:93:LYS:HZ2	1.63	0.46
1:C:171:ARG:HB2	1:C:272:TYR:HE1	1.81	0.45
1:B:48:TYR:CZ	1:B:184:HIS:HD2	2.34	0.45
1:A:197:ASN:ND2	1:A:197:ASN:N	2.53	0.45
1:B:30:LEU:HD22	1:B:291:VAL:HG21	1.98	0.45
1:A:255:THR:CG2	1:A:255:THR:O	2.63	0.45
1:A:275:GLU:OE2	1:B:114:GLN:O	2.35	0.45
1:A:97:TYR:CE1	1:A:113:VAL:HG22	2.52	0.45
1:A:275:GLU:OE2	1:B:114:GLN:C	2.60	0.45
1:B:39:ARG:CB	1:B:39:ARG:NH2	2.65	0.45
1:C:143:GLY:O	4:C:432:HOH:O	2.21	0.45
1:D:70:SER:O	1:D:234:LYS:HE3	2.17	0.45
1:C:240:ASP:O	1:C:243:ARG:HD2	2.17	0.45
1:D:241:TYR:HA	1:D:271:GLY:O	2.17	0.45
1:C:92:ASP:O	1:C:118:THR:HB	2.17	0.44
1:C:176:ASP:O	1:C:178:ARG:N	2.50	0.44
3:C:301:CD6:HAN	3:C:301:CD6:HNAS	1.77	0.44
4:B:421:HOH:O	1:D:33:ARG:HG2	2.16	0.44
1:C:98:THR:O	1:C:99:SER:C	2.61	0.44
1:A:87:PRO:O	1:A:88:LEU:C	2.61	0.44
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.70	0.44
1:B:240:ASP:O	1:B:241:TYR:HB2	2.18	0.44
3:C:301:CD6:HAN	3:C:301:CD6:CAP	2.47	0.44
1:D:76:LEU:O	1:D:79:ALA:HB3	2.17	0.44
1:C:97:TYR:CD2	1:C:97:TYR:N	2.86	0.44
1:D:257:VAL:HA	1:D:258:PRO:HD3	1.88	0.44
1:C:118:THR:H	1:C:121:GLN:HE21	1.65	0.43
3:B:301:CD6:OAE	3:B:301:CD6:CAA	2.30	0.43
1:C:93:LYS:O	1:C:118:THR:HA	2.17	0.43
1:A:275:GLU:HA	1:A:276:PRO:HD3	1.91	0.43
1:C:69:CYS:HB3	1:C:70:SER:H	1.65	0.43
1:C:166:ALA:HA	1:C:167:PRO:HA	1.77	0.43
3:C:301:CD6:HAN	3:C:301:CD6:HAP	1.99	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:37:LEU:O	1:D:41:TYR:HD1	2.01	0.43
1:A:46:GLY:HA2	1:A:60:TYR:O	2.19	0.43
1:D:90:HIS:HE1	1:D:141:ASP:OD2	2.01	0.43
1:D:178:ARG:O	1:D:179:ASP:HB2	2.19	0.43
1:B:176:ASP:C	1:B:176:ASP:OD2	2.61	0.43
1:D:246:ASP:OD2	4:D:422:HOH:O	2.21	0.43
1:A:172:ASP:HB2	4:A:407:HOH:O	2.19	0.43
1:B:88:LEU:O	1:B:91:LEU:HG	2.18	0.43
1:B:93:LYS:O	1:B:118:THR:HA	2.19	0.43
1:C:145(C):GLY:HA2	4:C:432:HOH:O	2.19	0.43
1:B:173:PRO:O	1:B:176:ASP:HB3	2.20	0.42
1:C:99:SER:OG	1:D:105:ILE:CA	2.66	0.42
1:B:105:ILE:HG22	1:B:107:PRO:HD3	2.01	0.42
1:C:76:LEU:HD12	1:C:76:LEU:O	2.18	0.42
1:A:112:HIS:HB3	1:A:115:THR:CG2	2.44	0.42
1:D:127:ILE:HG21	1:D:210:TRP:HB3	2.00	0.42
1:C:69:CYS:O	1:C:72:PHE:CD2	2.72	0.42
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.87	0.42
1:A:117:MET:HA	1:A:121:GLN:NE2	2.34	0.42
1:B:59:GLU:HB2	1:B:62:ALA:HB2	2.01	0.42
1:C:124:ASP:OD1	1:C:124:ASP:O	2.37	0.42
1:D:81:LEU:O	1:D:203:LYS:HD3	2.19	0.42
1:B:255:THR:HG22	1:B:255:THR:O	2.19	0.42
1:A:233:ASP:CB	1:A:248:ALA:HB2	2.50	0.42
1:D:270:GLY:HA3	1:D:274:ALA:HB2	2.02	0.42
1:B:222:ARG:NH2	1:B:226:PRO:O	2.53	0.42
1:B:238:GLY:HA2	3:B:301:CD6:HAPA	2.02	0.42
1:D:69:CYS:O	1:D:72:PHE:CD2	2.73	0.42
1:A:97:TYR:CE1	1:A:113:VAL:CG2	3.03	0.42
1:A:276:PRO:HD3	1:B:114:GLN:HB2	2.02	0.42
1:B:74:ALA:HB3	1:B:75:PRO:HD2	2.01	0.42
1:C:167:PRO:HG2	1:C:168:GLU:H	1.84	0.42
1:A:235:THR:HG22	1:A:246:ASP:OD1	2.20	0.41
1:C:161:ARG:O	1:C:161:ARG:HG3	2.20	0.41
1:D:93:LYS:HE3	1:D:93:LYS:HB2	1.58	0.41
1:D:228:ASP:OD1	1:D:228:ASP:N	2.53	0.41
1:D:67:ALA:HB3	1:D:243:ARG:HD3	2.01	0.41
1:D:74:ALA:HB3	1:D:75:PRO:CD	2.51	0.41
1:A:123:CYS:HB3	1:A:210:TRP:CZ3	2.55	0.41
1:C:197:ASN:H	1:C:197:ASN:HD22	1.69	0.41
1:A:106:SER:HB3	1:A:109:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLN:NE2	3:B:301:CD6:HAI	2.33	0.41
1:D:167:PRO:HD2	1:D:168:GLU:CD	2.46	0.41
1:A:68:PHE:CZ	1:A:181:THR:HB	2.56	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.57	0.41
1:A:153:ARG:HD3	1:A:157:ASP:O	2.21	0.41
1:C:97:TYR:OH	1:C:112:HIS:CB	2.67	0.41
1:C:74:ALA:HB3	1:C:75:PRO:HD3	2.03	0.41
1:D:168:GLU:CD	1:D:168:GLU:N	2.79	0.40
1:B:86:ASN:HB3	1:B:90:HIS:CB	2.51	0.40
1:D:115:THR:HG23	1:D:116:GLY:O	2.21	0.40
1:C:88:LEU:HD11	1:C:203:LYS:HG2	2.04	0.40
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.71	0.40
1:D:136:ASN:ND2	1:D:166:ALA:HB3	2.36	0.40
1:A:128:ARG:HG2	1:A:210:TRP:O	2.21	0.40
1:C:161:ARG:HD3	1:C:177:GLU:O	2.22	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	263/285 (92%)	253 (96%)	9 (3%)	1 (0%)	30	49
1	B	263/285 (92%)	254 (97%)	7 (3%)	2 (1%)	16	32
1	C	263/285 (92%)	240 (91%)	16 (6%)	7 (3%)	4	6
1	D	263/285 (92%)	248 (94%)	14 (5%)	1 (0%)	30	49
All	All	1052/1140 (92%)	995 (95%)	46 (4%)	11 (1%)	12	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	167	PRO
1	C	168	GLU
1	C	169	LEU
1	B	69	CYS
1	B	171	ARG
1	C	99	SER
1	C	173	PRO
1	C	177	GLU
1	A	69	CYS
1	C	69	CYS
1	D	69	CYS

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	201/218 (92%)	189 (94%)	12 (6%)	17	36
1	B	201/218 (92%)	186 (92%)	15 (8%)	12	26
1	C	200/218 (92%)	186 (93%)	14 (7%)	14	29
1	D	200/218 (92%)	190 (95%)	10 (5%)	22	44
All	All	802/872 (92%)	751 (94%)	51 (6%)	16	33

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	88	LEU
1	A	89	THR
1	A	111	GLN
1	A	113	VAL
1	A	115	THR
1	A	177	GLU
1	A	197	ASN
1	A	255	THR
1	A	277	ARG
1	A	280	LEU

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Mol	Chain	Res	Type
1	A	291	VAL
1	B	39	ARG
1	B	54	THR
1	B	68	PHE
1	B	71	THR
1	B	88	LEU
1	B	96	THR
1	B	102	ILE
1	B	115	THR
1	B	169	LEU
1	B	170	ASN
1	B	171	ARG
1	B	197	ASN
1	B	233	ASP
1	B	265	SER
1	B	280	LEU
1	C	39	ARG
1	C	68	PHE
1	C	88	LEU
1	C	89	THR
1	C	93	LYS
1	C	96	THR
1	C	102	ILE
1	C	106	SER
1	C	158	THR
1	C	169	LEU
1	C	170	ASN
1	C	197	ASN
1	C	280	LEU
1	C	291	VAL
1	D	89	THR
1	D	130	SER
1	D	169	LEU
1	D	186	ILE
1	D	197	ASN
1	D	215	THR
1	D	232	ILE
1	D	267	ARG
1	D	277	ARG
1	D	280	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	111	GLN
1	A	114	GLN
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	197	ASN
1	B	245	ASN
1	C	121	GLN
1	C	170	ASN
1	C	184	HIS
1	C	197	ASN
1	D	82	HIS
1	D	90	HIS
1	D	112	HIS
1	D	114	GLN
1	D	121	GLN
1	D	197	ASN

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](#)

9 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	PO4	A	301	-	4,4,4	3.05	4 (100%)	6,6,6	0.45	0
2	PO4	A	303	-	4,4,4	3.08	4 (100%)	6,6,6	0.46	0
2	PO4	D	302	-	4,4,4	3.07	4 (100%)	6,6,6	0.46	0
2	PO4	C	302	-	4,4,4	3.08	4 (100%)	6,6,6	0.46	0
2	PO4	B	302	-	4,4,4	3.06	4 (100%)	6,6,6	0.45	0
2	PO4	D	301	-	4,4,4	3.04	4 (100%)	6,6,6	0.45	0
3	CD6	B	301	1	21,24,24	3.22	6 (28%)	21,32,32	2.12	1 (4%)
3	CD6	C	301	1	21,24,24	3.22	5 (23%)	21,32,32	2.08	1 (4%)
2	PO4	A	302	-	4,4,4	3.05	4 (100%)	6,6,6	0.45	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
3	CD6	C	301	1	-	1/11/31/31	0/1/2/2
3	CD6	B	301	1	-	1/11/31/31	0/1/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	CD6	CAN-CAW	-8.27	1.39	1.50
3	C	301	CD6	CAN-CAW	-8.22	1.39	1.50
3	B	301	CD6	CAP-CBB	-7.61	1.39	1.51
3	C	301	CD6	CAP-CBB	-7.57	1.39	1.51
3	C	301	CD6	CBA-NAQ	6.87	1.34	1.28
3	B	301	CD6	CBA-NAQ	6.85	1.34	1.28
2	D	302	PO4	P-O1	4.71	1.61	1.50
2	A	303	PO4	P-O1	4.71	1.61	1.50
2	C	302	PO4	P-O1	4.71	1.61	1.50
2	B	302	PO4	P-O1	4.68	1.61	1.50
2	A	301	PO4	P-O1	4.64	1.61	1.50
2	A	302	PO4	P-O1	4.63	1.61	1.50
2	D	301	PO4	P-O1	4.63	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	CD6	CBA-CAX	-4.60	1.39	1.48
3	B	301	CD6	CBA-CAX	-4.59	1.39	1.48
3	C	301	CD6	CAA-CAW	3.38	1.39	1.32
3	B	301	CD6	CAA-CAW	3.32	1.39	1.32
2	A	303	PO4	P-O3	2.38	1.61	1.54
2	A	301	PO4	P-O3	2.37	1.61	1.54
2	A	302	PO4	P-O3	2.37	1.61	1.54
2	C	302	PO4	P-O2	2.37	1.61	1.54
2	D	301	PO4	P-O2	2.36	1.61	1.54
2	B	302	PO4	P-O3	2.36	1.61	1.54
2	C	302	PO4	P-O3	2.35	1.61	1.54
2	A	301	PO4	P-O2	2.35	1.61	1.54
2	A	302	PO4	P-O2	2.34	1.61	1.54
2	A	303	PO4	P-O2	2.34	1.61	1.54
2	D	302	PO4	P-O3	2.33	1.61	1.54
2	D	301	PO4	P-O3	2.33	1.61	1.54
2	B	302	PO4	P-O2	2.32	1.61	1.54
2	D	302	PO4	P-O2	2.32	1.61	1.54
2	A	303	PO4	P-O4	-2.16	1.48	1.54
2	C	302	PO4	P-O4	-2.15	1.48	1.54
2	A	302	PO4	P-O4	-2.14	1.48	1.54
2	D	302	PO4	P-O4	-2.14	1.48	1.54
2	B	302	PO4	P-O4	-2.12	1.48	1.54
2	D	301	PO4	P-O4	-2.12	1.48	1.54
2	A	301	PO4	P-O4	-2.11	1.48	1.54
3	B	301	CD6	CBA-CAW	-2.00	1.40	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	CD6	CBD-NAQ-CBA	8.80	124.01	116.33
3	C	301	CD6	CBD-NAQ-CBA	8.60	123.84	116.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

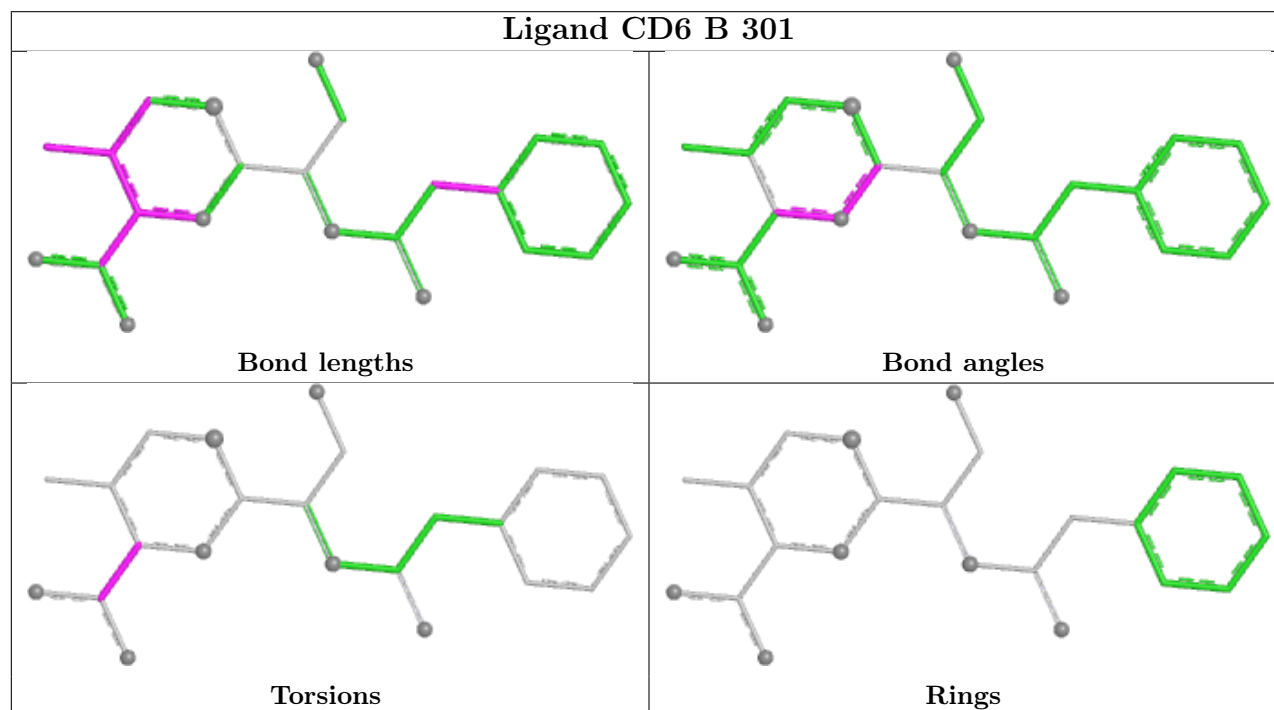
Mol	Chain	Res	Type	Atoms
3	B	301	CD6	OAH-CAX-CBA-CAW
3	C	301	CD6	OAH-CAX-CBA-CAW

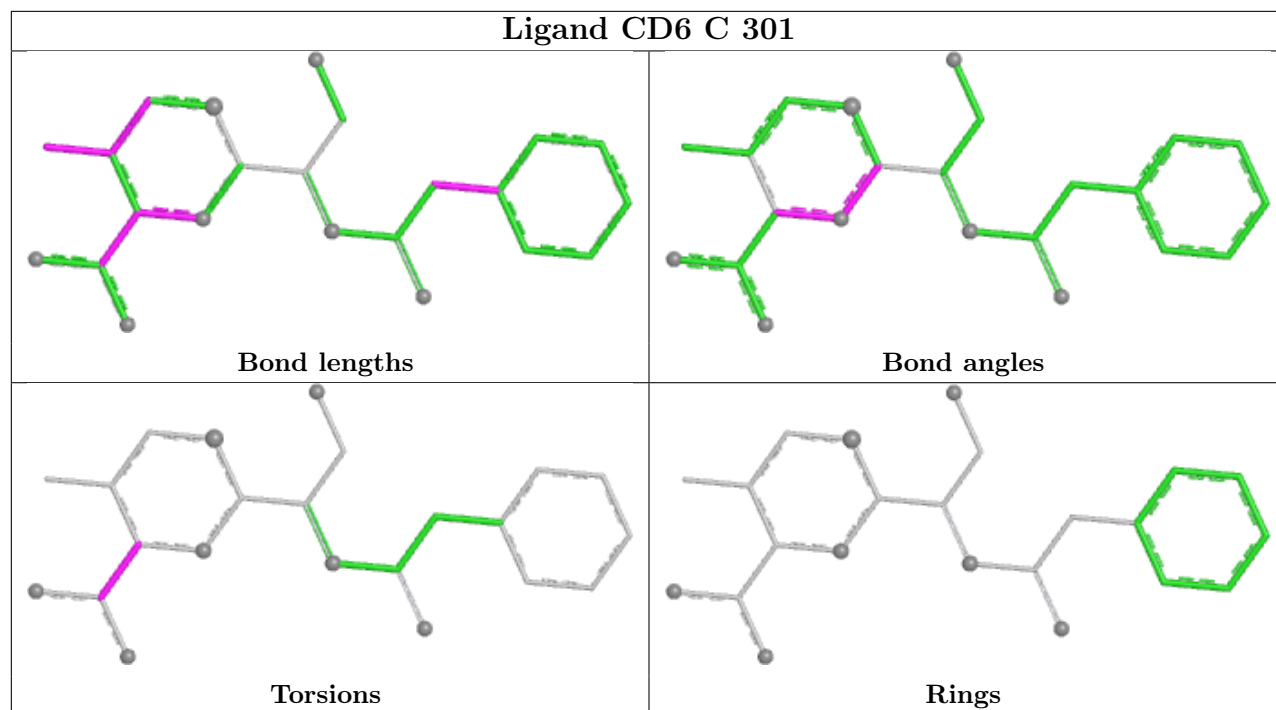
There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	PO4	1	0
2	D	301	PO4	2	0
3	B	301	CD6	15	0
3	C	301	CD6	10	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.





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%)	0.71	29 (10%) 10 9	25, 43, 74, 118	0
1	B	265/285 (92%)	0.66	32 (12%) 8 7	23, 44, 82, 118	0
1	C	265/285 (92%)	0.75	32 (12%) 8 7	23, 46, 86, 117	0
1	D	265/285 (92%)	0.75	32 (12%) 8 7	27, 47, 83, 107	0
All	All	1060/1140 (92%)	0.71	125 (11%) 9 7	23, 45, 82, 118	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	ASN	5.9
1	A	270	GLY	5.6
1	C	99	SER	5.5
1	C	89	THR	4.7
1	C	114	GLN	4.7
1	D	29	ASP	4.4
1	A	104	SER	4.3
1	C	167	PRO	4.2
1	D	104	SER	4.0
1	D	99	SER	3.9
1	D	39	ARG	3.6
1	C	166	ALA	3.6
1	B	272	TYR	3.6
1	A	103	ARG	3.6
1	B	173	PRO	3.6
1	C	103	ARG	3.6
1	C	100	ASP	3.6
1	C	113	VAL	3.5
1	A	275	GLU	3.5
1	D	270	GLY	3.5
1	C	168	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	164	ALA	3.4
1	B	29	ASP	3.3
1	B	172	ASP	3.3
1	B	99	SER	3.3
1	A	174	PRO	3.2
1	D	178	ARG	3.1
1	A	116	GLY	3.1
1	A	271	GLY	3.1
1	C	255	THR	3.1
1	C	157	ASP	3.1
1	A	102	ILE	3.1
1	B	166	ALA	3.0
1	D	166	ALA	3.0
1	B	167	PRO	3.0
1	B	169	LEU	3.0
1	B	157	ASP	3.0
1	D	269	GLY	2.9
1	B	54	THR	2.9
1	A	268	ALA	2.9
1	A	99	SER	2.8
1	D	110	GLN	2.8
1	B	53	GLY	2.8
1	B	43	ALA	2.7
1	B	174	PRO	2.7
1	B	36	GLU	2.7
1	A	29	ASP	2.7
1	C	98	THR	2.7
1	D	96	THR	2.7
1	A	276	PRO	2.7
1	C	169	LEU	2.6
1	A	164	ALA	2.6
1	D	255	THR	2.6
1	B	145(B)	GLY	2.6
1	C	29	ASP	2.6
1	A	105	ILE	2.6
1	C	110	GLN	2.5
1	B	146	ALA	2.5
1	C	272	TYR	2.5
1	A	115	THR	2.5
1	B	273	ASP	2.5
1	D	273	ASP	2.5
1	D	33	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	98	THR	2.5
1	A	33	ARG	2.4
1	A	168	GLU	2.4
1	D	115	THR	2.4
1	C	97	TYR	2.4
1	A	269	GLY	2.4
1	D	145(B)	GLY	2.4
1	B	171	ARG	2.4
1	D	93	LYS	2.4
1	B	89	THR	2.3
1	C	94	LEU	2.3
1	D	174	PRO	2.3
1	C	91	LEU	2.3
1	B	42	ASP	2.3
1	B	170	ASN	2.3
1	D	94	LEU	2.3
1	C	56	ALA	2.3
1	D	197	ASN	2.3
1	C	92	ASP	2.3
1	D	159	VAL	2.3
1	D	109	ALA	2.2
1	C	177	GLU	2.2
1	D	103	ARG	2.2
1	A	197	ASN	2.2
1	C	111	GLN	2.2
1	A	93	LYS	2.2
1	D	105	ILE	2.2
1	D	113	VAL	2.2
1	C	140	ALA	2.2
1	A	132	GLY	2.2
1	C	116	GLY	2.2
1	B	163	ASP	2.2
1	B	275	GLU	2.2
1	A	167	PRO	2.2
1	C	197	ASN	2.2
1	C	96	THR	2.2
1	B	103	ARG	2.2
1	D	116	GLY	2.1
1	B	102	ILE	2.1
1	C	105	ILE	2.1
1	A	177	GLU	2.1
1	B	178	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	293	ALA	2.1
1	B	129	TYR	2.1
1	A	69	CYS	2.1
1	D	111	GLN	2.1
1	D	114	GLN	2.1
1	D	126	ALA	2.1
1	B	158	THR	2.1
1	D	89	THR	2.1
1	C	39	ARG	2.1
1	D	119	ILE	2.1
1	A	101	ASP	2.1
1	A	210	TRP	2.1
1	B	145(C)	GLY	2.1
1	B	230	LYS	2.1
1	A	126	ALA	2.0
1	B	156	GLY	2.0
1	D	271	GLY	2.0
1	D	31	ALA	2.0
1	A	89	THR	2.0
1	C	102	ILE	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
3	CD6	C	301	23/23	0.77	0.27	42,83,123,125	0
3	CD6	B	301	23/23	0.79	0.24	42,80,127,159	0
2	PO4	C	302	5/5	0.83	0.10	76,76,94,95	0

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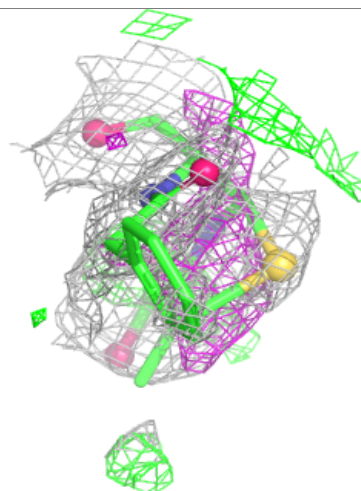
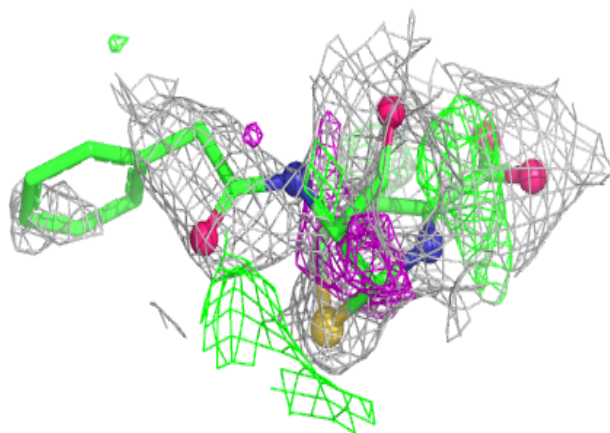
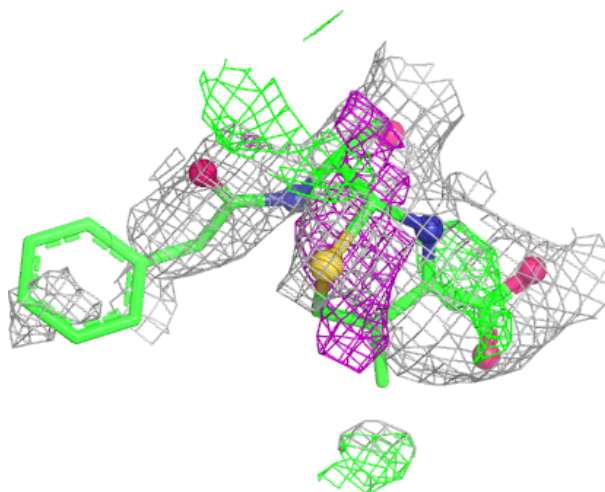
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	D	302	5/5	0.88	0.14	86,87,89,102	0
2	PO4	B	302	5/5	0.89	0.14	54,64,80,81	0
2	PO4	A	303	5/5	0.90	0.15	84,90,101,187	0
2	PO4	A	302	5/5	0.90	0.12	48,63,92,94	0
2	PO4	D	301	5/5	0.94	0.13	40,50,78,107	0
2	PO4	A	301	5/5	0.97	0.09	31,36,62,66	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.

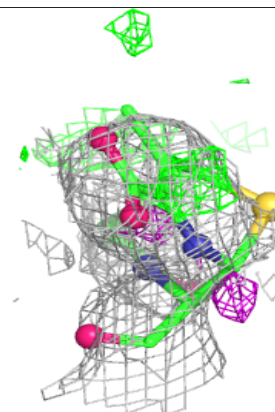
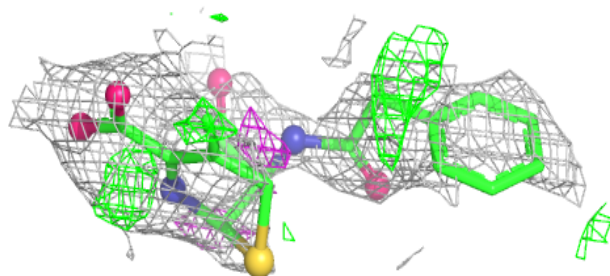
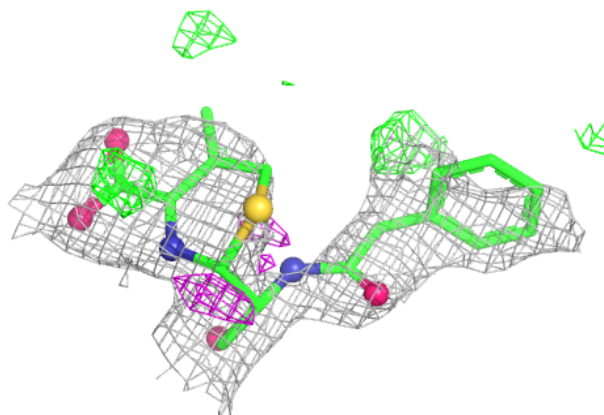
Electron density around CD6 C 301:

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 CD6 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.