Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 10:19 PM EDT

PDB ID	:	3L7M
Title	:	Structure of the Wall Teichoic Acid Polymerase TagF, H548A
Authors	:	Lovering, A.L.; Strynadka, N.C.J.
Deposited on	:	2009-12-28
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

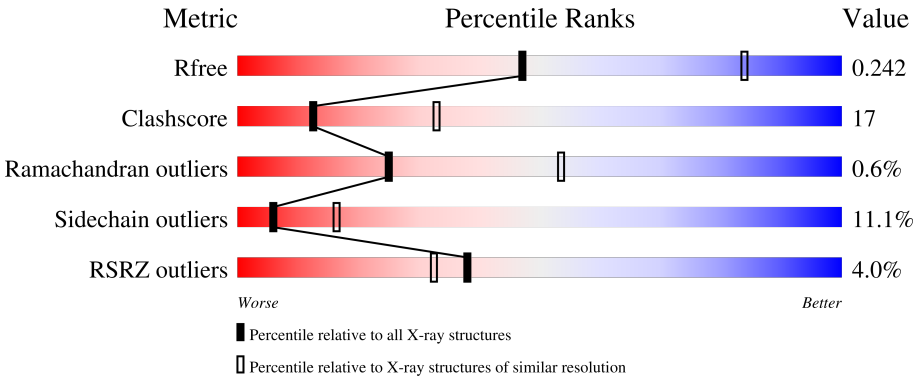
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	729	2% 35% 18% · 44%
1	B	729	2% 37% 16% · 44%
1	C	729	3% 36% 18% · 44%
1	D	729	3% 35% 19% · 43%

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
3	CL	A	735	-	-	-	X
3	CL	A	736	-	-	-	X
3	CL	B	733	-	-	-	X
3	CL	B	734	-	-	-	X
3	CL	B	735	-	-	X	-
3	CL	B	736	-	-	X	-
4	EDT	A	738	-	-	X	-
4	EDT	D	735	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13942 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 Teichoic acid biosynthesis protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3434	2206	572	645	11			
1	B	411	Total	C	N	O	S	0	0	0
			3464	2226	577	650	11			
1	C	411	Total	C	N	O	S	0	0	0
			3464	2226	577	650	11			
1	D	412	Total	C	N	O	S	0	0	0
			3474	2232	580	651	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	584	ALA	HIS	engineered mutation	UNP Q5HLM5
A	722	LEU	-	expression tag	UNP Q5HLM5
A	723	GLU	-	expression tag	UNP Q5HLM5
A	724	HIS	-	expression tag	UNP Q5HLM5
A	725	HIS	-	expression tag	UNP Q5HLM5
A	726	HIS	-	expression tag	UNP Q5HLM5
A	727	HIS	-	expression tag	UNP Q5HLM5
A	728	HIS	-	expression tag	UNP Q5HLM5
A	729	HIS	-	expression tag	UNP Q5HLM5
B	584	ALA	HIS	engineered mutation	UNP Q5HLM5
B	722	LEU	-	expression tag	UNP Q5HLM5
B	723	GLU	-	expression tag	UNP Q5HLM5
B	724	HIS	-	expression tag	UNP Q5HLM5
B	725	HIS	-	expression tag	UNP Q5HLM5
B	726	HIS	-	expression tag	UNP Q5HLM5
B	727	HIS	-	expression tag	UNP Q5HLM5
B	728	HIS	-	expression tag	UNP Q5HLM5
B	729	HIS	-	expression tag	UNP Q5HLM5
C	584	ALA	HIS	engineered mutation	UNP Q5HLM5
C	722	LEU	-	expression tag	UNP Q5HLM5
C	723	GLU	-	expression tag	UNP Q5HLM5

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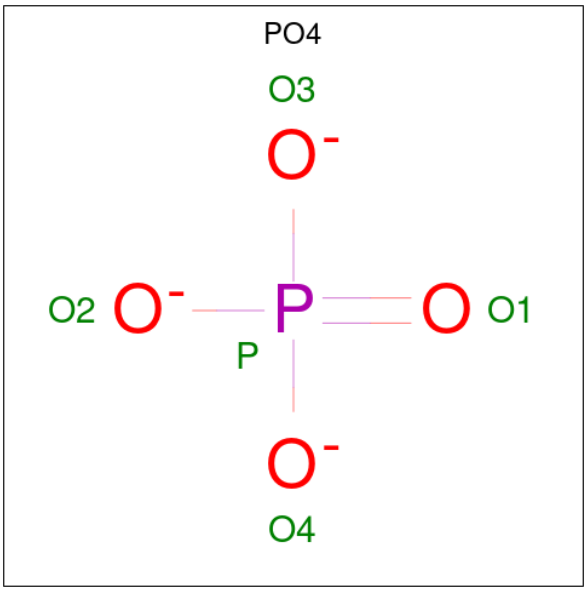
Chain	Residue	Modelled	Actual	Comment	Reference
C	724	HIS	-	expression tag	UNP Q5HLM5
C	725	HIS	-	expression tag	UNP Q5HLM5
C	726	HIS	-	expression tag	UNP Q5HLM5
C	727	HIS	-	expression tag	UNP Q5HLM5
C	728	HIS	-	expression tag	UNP Q5HLM5
C	729	HIS	-	expression tag	UNP Q5HLM5
D	584	ALA	HIS	engineered mutation	UNP Q5HLM5
D	722	LEU	-	expression tag	UNP Q5HLM5
D	723	GLU	-	expression tag	UNP Q5HLM5
D	724	HIS	-	expression tag	UNP Q5HLM5
D	725	HIS	-	expression tag	UNP Q5HLM5
D	726	HIS	-	expression tag	UNP Q5HLM5
D	727	HIS	-	expression tag	UNP Q5HLM5
D	728	HIS	-	expression tag	UNP Q5HLM5
D	729	HIS	-	expression tag	UNP Q5HLM5

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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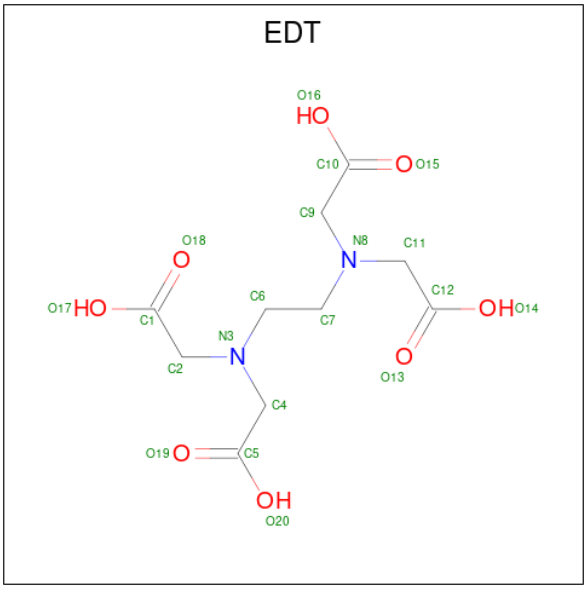
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Cl 6 6	0	0
3	B	6	Total Cl 6 6	0	0
3	C	2	Total Cl 2 2	0	0
3	D	4	Total Cl 4 4	0	0

- Molecule 4 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: $C_{10}H_{16}N_2O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 10 2 8	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			20	10	2	8		

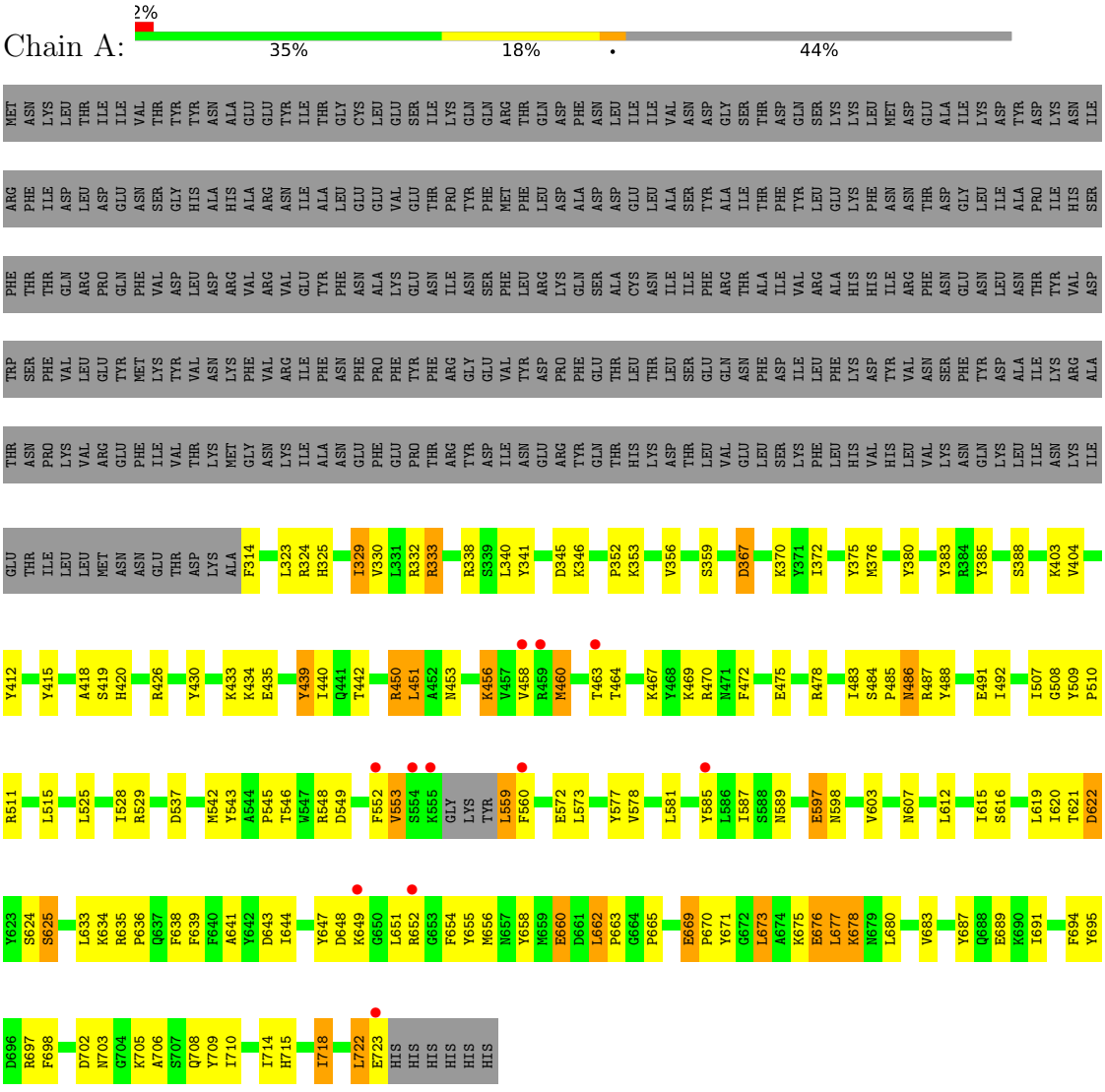
- Molecule 5 is water.

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

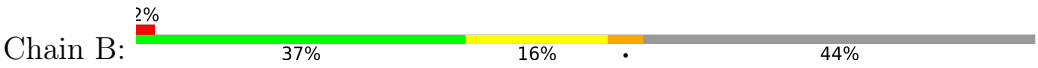
3 Residue-property plots (i)

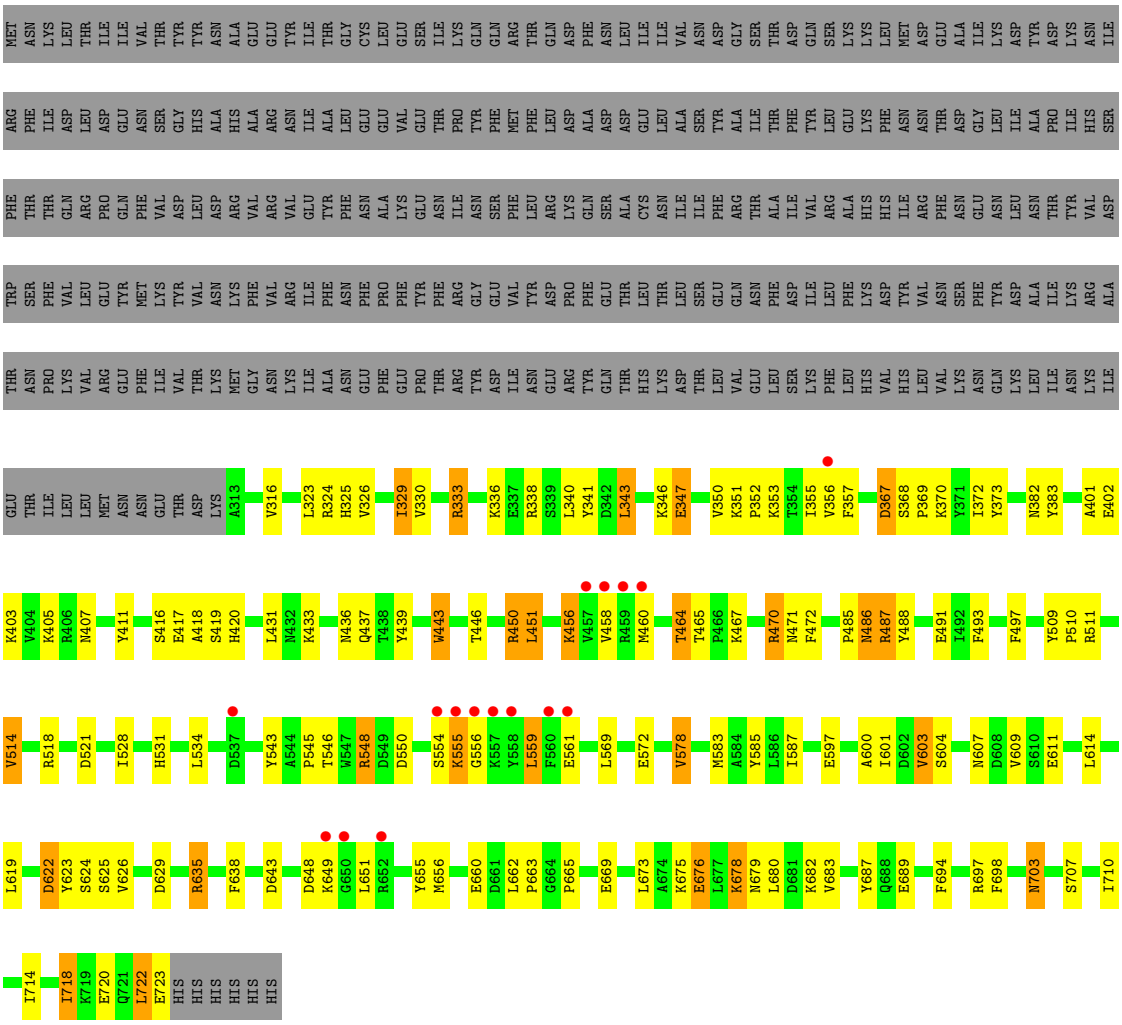
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Teichoic acid biosynthesis protein F



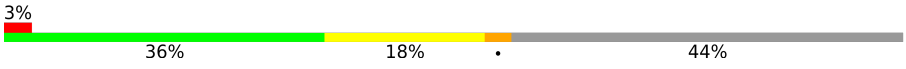
• Molecule 1: Teichoic acid biosynthesis protein F

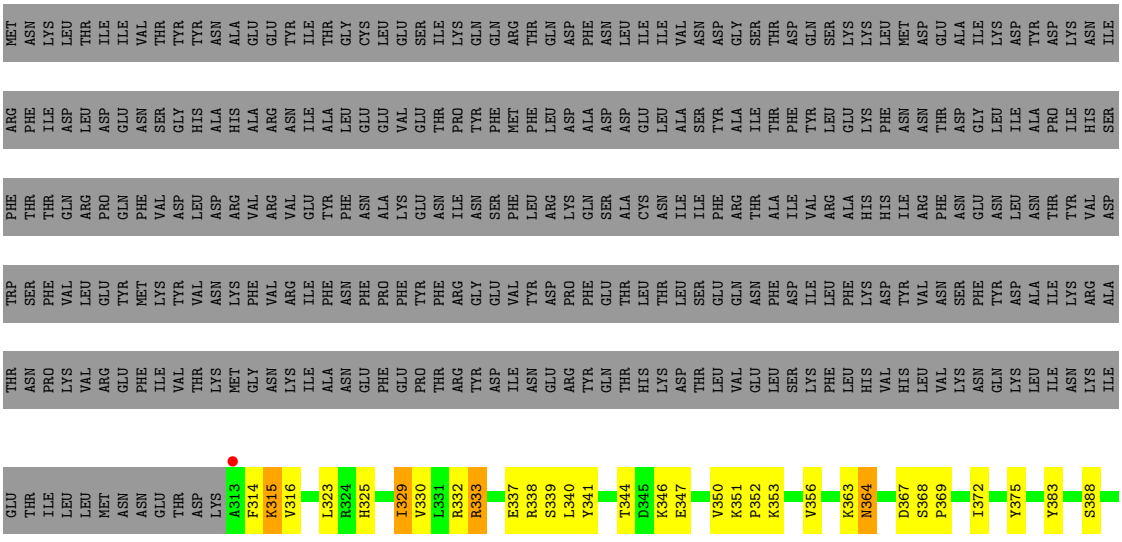


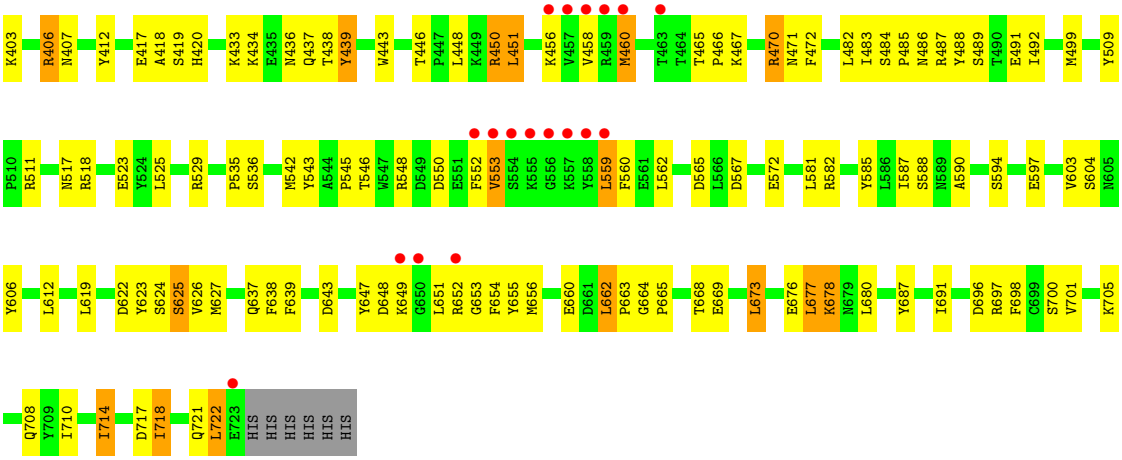


• Molecule 1: Teichoic acid biosynthesis protein F

Chain C:

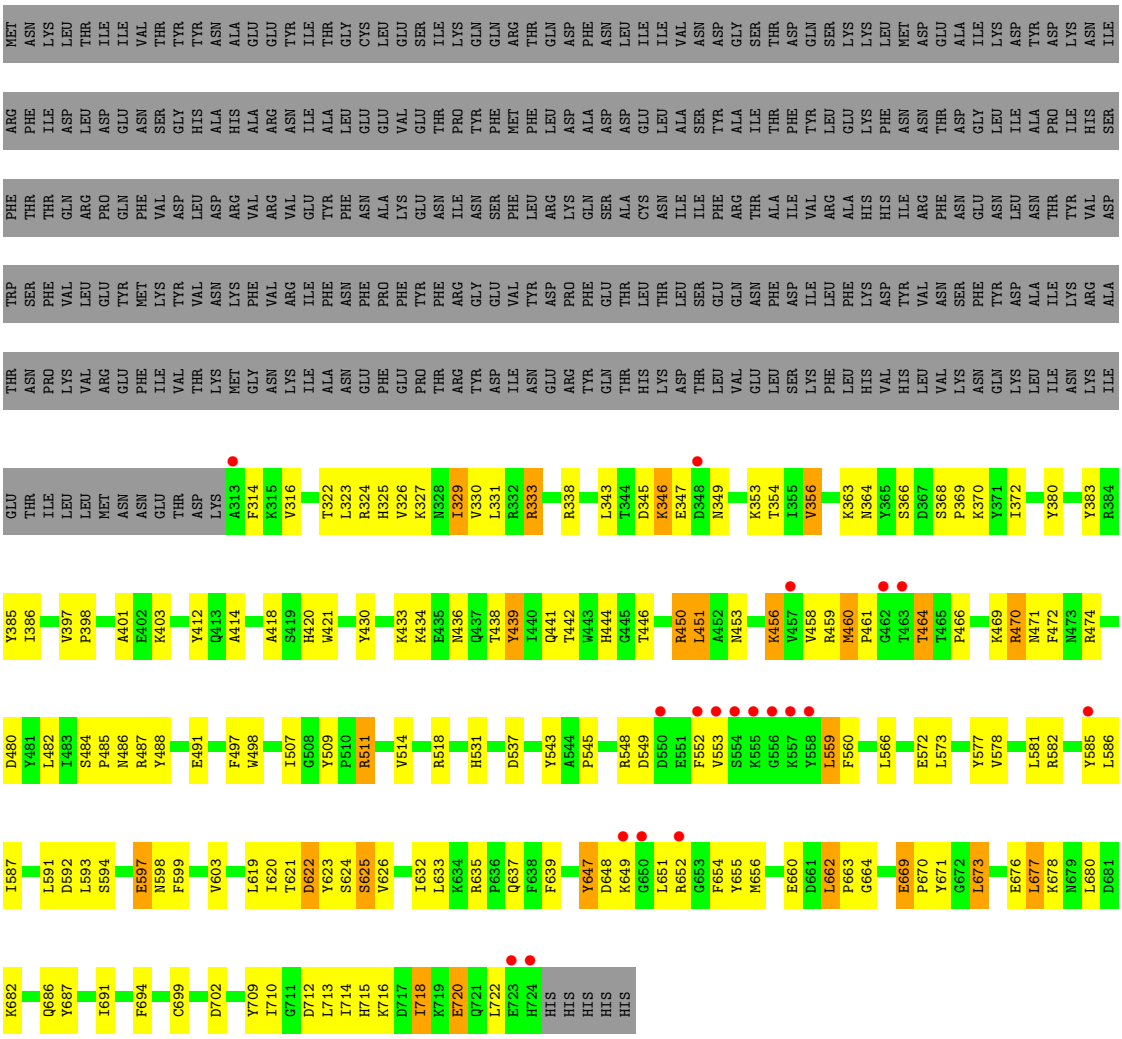






• Molecule 1: Teichoic acid biosynthesis protein F

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.51Å 223.51Å 101.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.85 19.94 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.94-2.85) 89.9 (19.94-2.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.251 0.185 , 0.242	Depositor DCC
R_{free} test set	2715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	86.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13942	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDT, CL, 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	0.41	0/3521	0.59	0/4757
1	B	0.43	0/3553	0.60	1/4801 (0.0%)
1	C	0.40	0/3553	0.58	0/4801
1	D	0.39	0/3564	0.59	0/4816
All	All	0.41	0/14191	0.59	1/19175 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	619	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	364	ASN	Peptide

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	3434	0	3342	121	0
1	B	3464	0	3373	103	0
1	C	3464	0	3373	118	0
1	D	3474	0	3380	123	0
2	A	10	0	0	1	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	6	0	0	2	0
3	B	6	0	0	5	0
3	C	2	0	0	1	0
3	D	4	0	0	2	0
4	A	20	0	16	10	0
4	D	20	0	16	7	0
5	A	1	0	0	0	0
5	B	4	0	0	2	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
All	All	13942	0	13500	462	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 17.

All (462) 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:470:ARG:HH11	1:C:470:ARG:HG2	1.10	1.10
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.20	1.04
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.19	1.00
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.21	1.00
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.21	0.99
1:A:442:THR:HG22	1:A:483:ILE:HD12	1.43	0.99
1:C:485:PRO:HG3	1:C:509:TYR:CE2	2.01	0.96
1:A:353:LYS:HG2	3:A:732:CL:CL	2.02	0.95
1:D:324:ARG:HD3	4:D:735:EDT:H022	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.33	0.92
1:A:324:ARG:HD3	4:A:738:EDT:H091	1.53	0.91
1:C:372:ILE:HD13	1:C:710:ILE:HG21	1.54	0.88
1:D:543:TYR:CZ	1:D:545:PRO:HG3	2.09	0.87
1:A:648:ASP:HB2	1:A:651:LEU:HB3	1.54	0.87
1:C:648:ASP:HB2	1:C:651:LEU:HB3	1.56	0.85
1:D:485:PRO:HG3	1:D:509:TYR:CE2	2.13	0.84
1:C:333:ARG:HH11	1:C:333:ARG:CG	1.92	0.82
1:A:383:TYR:CE2	1:A:718:ILE:HD11	2.14	0.81
1:B:648:ASP:HB2	1:B:651:LEU:HB3	1.62	0.81
1:B:383:TYR:CE2	1:B:718:ILE:HD11	2.16	0.81
1:D:383:TYR:CE2	1:D:718:ILE:HD11	2.16	0.81
1:B:372:ILE:HD13	1:B:710:ILE:HG21	1.63	0.79
1:B:353:LYS:HG2	3:B:733:CL:CL	2.19	0.79
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.46	0.79
1:C:662:LEU:CD2	1:C:662:LEU:H	1.95	0.78
1:D:548:ARG:HH22	1:D:622:ASP:CG	1.86	0.78
1:C:543:TYR:CE2	1:C:545:PRO:HG3	2.19	0.78
1:D:353:LYS:HG2	3:D:732:CL:CL	2.20	0.78
1:A:714:ILE:O	1:A:718:ILE:HG23	1.85	0.77
1:B:333:ARG:HG2	1:B:333:ARG:NH1	1.97	0.77
1:A:451:LEU:H	1:A:451:LEU:HD12	1.50	0.77
1:B:451:LEU:HD12	1:B:451:LEU:H	1.50	0.77
1:B:543:TYR:CZ	1:B:545:PRO:HG3	2.20	0.76
1:C:543:TYR:CZ	1:C:545:PRO:HG3	2.19	0.76
1:D:572:GLU:OE1	1:D:678:LYS:HE3	1.87	0.75
1:A:324:ARG:HD3	4:A:738:EDT:C9	2.17	0.75
1:B:456:LYS:HA	1:B:456:LYS:HE2	1.68	0.74
1:C:662:LEU:H	1:C:662:LEU:HD23	1.51	0.74
1:D:324:ARG:HH11	4:D:735:EDT:H022	1.53	0.74
1:B:722:LEU:O	1:B:723:GLU:HG3	1.88	0.72
1:B:624:SER:OG	1:B:626:VAL:HG22	1.90	0.71
1:D:451:LEU:HD12	1:D:451:LEU:H	1.55	0.71
1:A:542:MET:HE1	1:A:612:LEU:HB3	1.71	0.71
1:D:433:LYS:HD2	1:D:439:TYR:HB2	1.73	0.70
1:D:347:GLU:HG3	1:D:436:ASN:HB2	1.74	0.70
1:C:665:PRO:HG3	1:C:687:TYR:CE1	2.26	0.69
1:B:561:GLU:HB2	3:B:735:CL:CL	2.30	0.69
1:C:639:PHE:CZ	1:C:663:PRO:HD2	2.28	0.69
1:A:722:LEU:O	1:A:723:GLU:HG3	1.93	0.68
1:B:511:ARG:HH22	1:B:629:ASP:CG	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:HH11	1:C:333:ARG:HG2	1.57	0.68
1:B:470:ARG:HG2	1:B:470:ARG:NH1	1.95	0.68
1:D:372:ILE:HD13	1:D:710:ILE:HG21	1.75	0.68
1:A:485:PRO:HG3	1:A:509:TYR:CE2	2.29	0.68
1:A:356:VAL:HG11	1:A:415:TYR:CZ	2.29	0.68
1:D:673:LEU:HD22	1:D:677:LEU:HD22	1.77	0.67
1:D:450:ARG:HA	1:D:655:TYR:CE2	2.29	0.67
1:A:456:LYS:HE2	1:A:456:LYS:HA	1.74	0.67
1:D:470:ARG:HG2	1:D:470:ARG:NH1	1.97	0.67
1:A:470:ARG:HG2	1:A:470:ARG:NH1	2.01	0.66
1:D:714:ILE:O	1:D:718:ILE:HG23	1.95	0.66
1:A:508:GLY:HA3	1:A:702:ASP:OD1	1.95	0.66
1:D:446:THR:O	1:D:625:SER:HB2	1.96	0.66
1:C:470:ARG:HG2	1:C:470:ARG:NH1	1.89	0.66
1:B:548:ARG:HD3	1:B:643:ASP:OD2	1.95	0.66
1:A:356:VAL:HG23	1:A:418:ALA:HB2	1.78	0.66
1:B:548:ARG:HH22	1:B:622:ASP:CG	1.98	0.66
1:A:572:GLU:O	1:A:573:LEU:HD23	1.96	0.66
1:C:446:THR:O	1:C:625:SER:HB2	1.96	0.65
1:A:467:LYS:HE3	1:A:470:ARG:NH2	2.11	0.65
1:B:514:VAL:HG12	1:B:518:ARG:HG3	1.77	0.65
1:A:652:ARG:C	1:A:654:PHE:H	2.00	0.65
1:D:327:LYS:NZ	4:D:735:EDT:H062	2.11	0.64
1:B:559:LEU:HD23	1:B:587:ILE:HG23	1.79	0.64
1:A:543:TYR:CZ	1:A:545:PRO:HG3	2.32	0.64
1:C:347:GLU:HG3	1:C:436:ASN:HB2	1.79	0.64
1:B:458:VAL:HG13	1:B:460:MET:HG2	1.80	0.64
1:C:356:VAL:HG23	1:C:418:ALA:HB2	1.80	0.64
1:D:453:ASN:HB2	1:D:498:TRP:CZ2	2.33	0.64
1:A:488:TYR:OH	1:A:655:TYR:HB2	1.98	0.63
1:A:467:LYS:HE3	1:A:470:ARG:HH22	1.62	0.63
1:D:456:LYS:HE2	1:D:456:LYS:HA	1.80	0.63
1:D:624:SER:OG	1:D:626:VAL:HG22	1.99	0.62
1:A:333:ARG:HG2	1:A:333:ARG:NH1	1.97	0.62
1:B:703:ASN:H	1:B:703:ASN:ND2	1.95	0.62
1:C:351:LYS:HD2	1:C:417:GLU:OE1	1.99	0.62
1:A:543:TYR:CE2	1:A:545:PRO:HG3	2.34	0.62
1:A:665:PRO:HG3	1:A:687:TYR:CE1	2.35	0.62
1:A:647:TYR:O	1:A:651:LEU:HD22	1.99	0.62
1:A:338:ARG:NH1	1:A:430:TYR:CZ	2.68	0.61
1:A:634:LYS:HE3	1:A:695:TYR:CG	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:PRO:HG3	1:B:509:TYR:CE2	2.35	0.61
1:B:625:SER:N	2:B:731:PO4:O2	2.25	0.61
1:D:322:THR:O	1:D:326:VAL:HG23	2.01	0.61
1:D:453:ASN:HA	1:D:469:LYS:HD3	1.82	0.61
1:A:353:LYS:HB2	1:A:383:TYR:HD2	1.66	0.61
1:A:548:ARG:NH2	1:A:622:ASP:OD1	2.25	0.61
1:B:403:LYS:HE2	3:B:736:CL:CL	2.37	0.61
1:C:347:GLU:O	1:C:436:ASN:ND2	2.33	0.61
1:B:433:LYS:HE3	1:B:437:GLN:O	2.01	0.61
1:A:451:LEU:HD12	1:A:451:LEU:N	2.15	0.61
1:B:663:PRO:HG3	1:B:694:PHE:CG	2.36	0.61
1:B:675:LYS:O	1:B:678:LYS:HB2	2.01	0.61
1:C:548:ARG:HD3	1:C:643:ASP:OD2	2.00	0.60
1:D:670:PRO:HD2	1:D:671:TYR:CD2	2.36	0.60
1:B:347:GLU:O	1:B:436:ASN:ND2	2.34	0.60
1:D:453:ASN:HB2	1:D:498:TRP:CH2	2.37	0.60
1:B:446:THR:O	1:B:625:SER:HB2	2.02	0.60
1:B:665:PRO:HG3	1:B:687:TYR:OH	2.02	0.60
1:D:338:ARG:HD2	1:D:430:TYR:CD1	2.36	0.60
1:C:333:ARG:HG2	1:C:333:ARG:NH1	2.16	0.59
1:B:416:SER:HA	5:B:740:HOH:O	2.00	0.59
1:C:333:ARG:HH11	1:C:333:ARG:HG3	1.67	0.59
1:D:582:ARG:HD3	3:D:734:CL:CL	2.39	0.59
1:B:458:VAL:CG1	1:B:460:MET:HG2	2.33	0.59
1:C:467:LYS:HE3	1:C:470:ARG:HH22	1.67	0.59
1:B:572:GLU:OE1	1:B:678:LYS:HE3	2.03	0.59
1:A:324:ARG:CD	4:A:738:EDT:H091	2.30	0.59
1:C:485:PRO:HG3	1:C:509:TYR:HE2	1.65	0.59
1:A:324:ARG:HD2	4:A:738:EDT:O14	2.02	0.59
1:A:478:ARG:HD2	3:A:736:CL:CL	2.40	0.59
1:A:662:LEU:HB2	1:A:663:PRO:HD3	1.84	0.59
1:A:648:ASP:CB	1:A:651:LEU:HB3	2.30	0.59
1:A:548:ARG:HD3	1:A:643:ASP:OD2	2.03	0.58
1:B:485:PRO:HB2	1:B:486:ASN:ND2	2.18	0.58
1:D:464:THR:OG1	1:D:466:PRO:HD2	2.03	0.58
1:A:703:ASN:HB2	1:A:705:LYS:H	1.68	0.58
1:B:488:TYR:OH	1:B:655:TYR:HB2	2.03	0.58
1:C:316:VAL:HG23	1:D:331:LEU:CD2	2.33	0.58
1:A:665:PRO:HG3	1:A:687:TYR:CZ	2.39	0.58
1:B:418:ALA:O	1:B:437:GLN:HG2	2.04	0.58
1:C:552:PHE:O	1:C:553:VAL:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ILE:HD13	1:A:710:ILE:HG21	1.86	0.58
1:A:597:GLU:O	1:A:598:ASN:HB2	2.03	0.58
1:C:338:ARG:HD3	1:C:412:TYR:OH	2.03	0.57
1:A:625:SER:HB3	2:A:731:PO4:O4	2.04	0.57
1:C:673:LEU:HD22	1:C:677:LEU:HD22	1.86	0.57
1:B:714:ILE:O	1:B:718:ILE:HG23	2.04	0.57
1:B:648:ASP:O	1:B:649:LYS:HB2	2.03	0.57
1:B:346:LYS:CE	1:C:332:ARG:HH22	2.18	0.57
1:C:383:TYR:CE2	1:C:718:ILE:HD11	2.40	0.57
1:D:573:LEU:HB3	1:D:577:TYR:HD2	1.69	0.57
1:B:356:VAL:HG23	1:B:418:ALA:CB	2.34	0.57
1:C:325:HIS:NE2	1:C:329:ILE:HD13	2.19	0.57
1:C:652:ARG:C	1:C:654:PHE:H	2.08	0.56
1:C:488:TYR:O	1:C:492:ILE:HG13	2.05	0.56
1:D:687:TYR:O	1:D:691:ILE:HG13	2.05	0.56
1:B:383:TYR:CZ	1:B:718:ILE:HD11	2.41	0.56
1:D:597:GLU:O	1:D:598:ASN:HB2	2.05	0.56
1:B:451:LEU:HD12	1:B:451:LEU:N	2.21	0.56
1:C:470:ARG:HH11	1:C:470:ARG:CG	2.00	0.56
1:A:485:PRO:HG3	1:A:509:TYR:CZ	2.41	0.56
1:A:673:LEU:HD22	1:A:677:LEU:HD22	1.88	0.56
1:D:442:THR:O	1:D:509:TYR:HE1	1.89	0.56
1:C:340:LEU:O	1:C:344:THR:HG23	2.06	0.55
1:D:663:PRO:HG3	1:D:694:PHE:CG	2.41	0.55
1:D:716:LYS:O	1:D:720:GLU:HG2	2.05	0.55
1:D:662:LEU:HB2	1:D:663:PRO:HD3	1.88	0.55
1:A:450:ARG:HA	1:A:655:TYR:CE2	2.42	0.55
1:C:420:HIS:CD2	1:C:438:THR:HB	2.41	0.55
4:A:738:EDT:C6	4:A:738:EDT:C10	2.85	0.55
1:C:341:TYR:CD1	1:C:412:TYR:HB3	2.42	0.55
1:A:663:PRO:HG3	1:A:694:PHE:CD2	2.42	0.55
1:B:356:VAL:HG23	1:B:418:ALA:HB2	1.89	0.54
1:D:470:ARG:HH11	1:D:470:ARG:CG	2.09	0.54
1:A:675:LYS:O	1:A:678:LYS:HB2	2.08	0.54
4:A:738:EDT:C1	4:A:738:EDT:C7	2.85	0.54
4:A:738:EDT:C1	1:B:324:ARG:HD3	2.38	0.54
1:C:363:LYS:HE2	1:C:364:ASN:ND2	2.22	0.54
1:A:621:THR:O	1:A:639:PHE:HA	2.07	0.54
1:B:648:ASP:CB	1:B:651:LEU:HB3	2.35	0.54
1:B:326:VAL:HG11	1:D:326:VAL:HG11	1.89	0.54
1:B:561:GLU:CB	3:B:735:CL:CL	2.93	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LYS:HD2	1:C:439:TYR:HB2	1.90	0.54
1:C:638:PHE:HE1	1:C:676:GLU:HG2	1.73	0.54
1:D:639:PHE:CZ	1:D:663:PRO:HD2	2.43	0.54
1:D:327:LYS:HZ1	4:D:735:EDT:H062	1.73	0.53
1:B:534:LEU:HD22	1:B:578:VAL:HG11	1.89	0.53
1:C:465:THR:HB	1:C:466:PRO:HD3	1.90	0.53
1:C:492:ILE:HD13	1:C:655:TYR:CD2	2.44	0.53
1:A:638:PHE:CZ	1:A:683:VAL:HG11	2.44	0.53
1:A:697:ARG:HD3	1:A:698:PHE:CZ	2.44	0.53
1:B:603:VAL:O	1:B:603:VAL:HG13	2.08	0.53
1:C:451:LEU:H	1:C:451:LEU:HD12	1.74	0.53
1:D:548:ARG:NH2	1:D:622:ASP:OD1	2.41	0.53
1:A:458:VAL:HG13	1:A:460:MET:CE	2.39	0.53
1:D:438:THR:HA	1:D:480:ASP:OD2	2.09	0.53
1:D:507:ILE:HD13	1:D:709:TYR:HD2	1.73	0.53
1:C:353:LYS:HA	1:C:718:ILE:HD12	1.90	0.53
1:B:601:ILE:HD13	1:B:601:ILE:N	2.23	0.52
1:C:486:ASN:OD1	1:C:488:TYR:HB3	2.09	0.52
1:D:625:SER:N	2:D:731:PO4:O1	2.37	0.52
1:D:338:ARG:HD3	1:D:412:TYR:OH	2.10	0.52
1:A:353:LYS:HB2	1:A:383:TYR:CD2	2.42	0.52
1:D:593:LEU:N	1:D:593:LEU:HD23	2.24	0.52
1:A:641:ALA:HB1	1:A:644:ILE:HB	1.92	0.52
1:A:453:ASN:HA	1:A:469:LYS:HD3	1.92	0.52
1:A:458:VAL:HG13	1:A:460:MET:HE2	1.92	0.52
1:A:662:LEU:H	1:A:662:LEU:CD2	2.23	0.52
1:D:347:GLU:CG	1:D:436:ASN:HB2	2.39	0.52
1:A:525:LEU:HD22	1:A:615:ILE:HG22	1.90	0.51
1:B:665:PRO:HG3	1:B:687:TYR:CZ	2.45	0.51
1:C:662:LEU:CD2	1:C:662:LEU:N	2.66	0.51
1:D:537:ASP:OD1	1:D:537:ASP:N	2.40	0.51
1:A:620:ILE:HD11	1:A:677:LEU:HD21	1.91	0.51
1:A:663:PRO:HG3	1:A:694:PHE:CG	2.46	0.51
1:C:337:GLU:OE1	1:C:337:GLU:HA	2.11	0.51
1:A:718:ILE:HG13	1:A:718:ILE:O	2.11	0.51
1:B:372:ILE:HD13	1:B:710:ILE:CG2	2.38	0.51
1:B:559:LEU:O	1:B:559:LEU:HD12	2.10	0.51
1:B:470:ARG:NH1	1:B:471:ASN:OD1	2.42	0.51
1:D:718:ILE:HG13	1:D:718:ILE:O	2.11	0.51
1:A:662:LEU:HB2	1:A:663:PRO:CD	2.41	0.51
1:C:648:ASP:HB2	1:C:651:LEU:CB	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:ARG:C	1:D:654:PHE:H	2.14	0.50
1:C:333:ARG:CG	1:C:333:ARG:NH1	2.60	0.50
1:C:546:THR:HG23	1:C:624:SER:HB2	1.91	0.50
1:A:676:GLU:HG3	1:A:683:VAL:HG22	1.94	0.50
1:B:368:SER:HB2	1:B:369:PRO:HD3	1.93	0.50
1:B:333:ARG:O	1:B:336:LYS:HG2	2.10	0.50
1:B:531:HIS:HD2	1:B:531:HIS:O	1.94	0.50
1:B:367:ASP:OD2	1:B:511:ARG:HD3	2.11	0.50
1:C:697:ARG:HD3	1:C:698:PHE:CE2	2.46	0.50
1:D:354:THR:HG22	1:D:418:ALA:HA	1.94	0.50
1:A:341:TYR:CD1	1:A:412:TYR:HB3	2.47	0.50
1:D:331:LEU:HB2	1:D:333:ARG:HD3	1.92	0.50
1:C:350:VAL:HA	1:C:417:GLU:O	2.12	0.49
1:C:352:PRO:O	1:C:718:ILE:HD12	2.11	0.49
1:C:458:VAL:HG13	1:C:460:MET:HE3	1.94	0.49
1:B:470:ARG:HH11	1:B:470:ARG:CG	2.07	0.49
1:D:637:GLN:O	1:D:664:GLY:HA3	2.12	0.49
1:C:637:GLN:O	1:C:664:GLY:HA3	2.12	0.49
1:D:327:LYS:HZ3	4:D:735:EDT:H062	1.78	0.49
1:D:514:VAL:HG12	1:D:518:ARG:HG3	1.94	0.49
1:B:420:HIS:CE1	1:B:718:ILE:HG22	2.48	0.49
1:C:624:SER:OG	1:C:626:VAL:HG13	2.12	0.49
1:B:638:PHE:HE1	1:B:676:GLU:HG2	1.78	0.49
1:C:325:HIS:HB2	1:C:339:SER:HB2	1.94	0.49
1:C:717:ASP:O	1:C:721:GLN:HG3	2.13	0.49
1:D:682:LYS:O	1:D:686:GLN:HB2	2.13	0.49
1:B:467:LYS:HE3	1:B:470:ARG:NH2	2.28	0.49
1:C:368:SER:HB2	1:C:369:PRO:HD3	1.94	0.49
1:D:444:HIS:C	1:D:511:ARG:NH1	2.67	0.49
1:D:497:PHE:O	1:D:498:TRP:HB2	2.11	0.49
1:D:592:ASP:C	1:D:593:LEU:HD23	2.33	0.49
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.69	0.48
1:A:488:TYR:O	1:A:492:ILE:HG13	2.12	0.48
1:A:542:MET:CE	1:A:612:LEU:HB3	2.39	0.48
1:D:543:TYR:CE2	1:D:545:PRO:HG3	2.48	0.48
1:C:714:ILE:O	1:C:718:ILE:HG22	2.14	0.48
1:D:578:VAL:HG23	1:D:599:PHE:HA	1.95	0.48
1:B:679:ASN:ND2	1:B:682:LYS:HB2	2.27	0.48
1:A:353:LYS:HA	1:A:718:ILE:HD12	1.95	0.48
1:C:458:VAL:HG13	1:C:460:MET:CE	2.43	0.48
1:D:682:LYS:HE3	1:D:682:LYS:HB2	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:PHE:O	1:D:553:VAL:HG13	2.14	0.48
1:D:662:LEU:HB2	1:D:663:PRO:CD	2.44	0.48
1:B:367:ASP:O	1:B:370:LYS:HB3	2.14	0.48
1:C:680:LEU:HD23	1:C:680:LEU:HA	1.64	0.48
1:D:383:TYR:CZ	1:D:718:ILE:HD11	2.48	0.48
1:A:345:ASP:OD1	1:A:434:LYS:HE3	2.14	0.48
1:A:442:THR:HG22	1:A:483:ILE:CD1	2.29	0.48
4:A:738:EDT:C1	4:A:738:EDT:H072	2.41	0.48
1:D:333:ARG:HG2	1:D:333:ARG:NH1	2.16	0.48
1:A:325:HIS:CE1	1:A:340:LEU:HB2	2.49	0.47
1:A:420:HIS:CD2	1:A:714:ILE:HG12	2.49	0.47
1:A:644:ILE:HG12	1:A:644:ILE:O	2.14	0.47
1:B:347:GLU:HG3	1:B:436:ASN:ND2	2.29	0.47
1:C:488:TYR:OH	1:C:655:TYR:HB2	2.12	0.47
1:C:517:ASN:C	1:C:518:ARG:HG2	2.34	0.47
1:D:345:ASP:OD1	1:D:434:LYS:HE3	2.13	0.47
1:D:485:PRO:HB2	1:D:486:ASN:ND2	2.28	0.47
1:D:368:SER:HB2	1:D:369:PRO:HD3	1.96	0.47
1:C:722:LEU:HD12	1:C:722:LEU:HA	1.75	0.47
1:C:582:ARG:O	1:C:582:ARG:CG	2.62	0.47
1:C:588:SER:C	1:C:590:ALA:H	2.18	0.47
1:B:559:LEU:CD2	1:B:587:ILE:HG23	2.43	0.47
1:C:344:THR:O	1:C:346:LYS:HG3	2.13	0.47
1:B:352:PRO:HA	1:B:419:SER:HB3	1.96	0.47
1:B:518:ARG:NH1	1:B:521:ASP:OD1	2.48	0.47
1:C:316:VAL:HG23	1:D:331:LEU:HD22	1.97	0.47
1:A:338:ARG:NH1	1:A:430:TYR:CE1	2.83	0.47
1:D:353:LYS:HA	1:D:718:ILE:HD12	1.97	0.47
1:A:345:ASP:OD1	1:A:434:LYS:CE	2.62	0.47
1:B:333:ARG:NH1	1:B:333:ARG:CG	2.72	0.46
1:C:542:MET:HB3	1:C:619:LEU:HD23	1.96	0.46
1:D:471:ASN:O	1:D:474:ARG:HB2	2.15	0.46
1:A:510:PRO:HA	1:A:706:ALA:HB3	1.97	0.46
1:A:559:LEU:HD23	1:A:587:ILE:HG23	1.96	0.46
1:D:356:VAL:HG23	1:D:421:TRP:HA	1.97	0.46
1:A:515:LEU:HD22	1:A:633:LEU:HD11	1.96	0.46
1:C:648:ASP:O	1:C:649:LYS:HB2	2.14	0.46
1:D:329:ILE:HG22	1:D:330:VAL:N	2.30	0.46
1:D:363:LYS:HG3	1:D:364:ASN:OD1	2.15	0.46
1:C:482:LEU:HD23	1:C:499:MET:HG3	1.96	0.46
1:C:559:LEU:CD1	1:C:559:LEU:C	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:HG22	1:A:330:VAL:N	2.30	0.46
1:A:662:LEU:H	1:A:662:LEU:HD23	1.79	0.46
1:B:346:LYS:HE3	1:C:332:ARG:HH22	1.79	0.46
1:A:636:PRO:HA	1:A:691:ILE:HD11	1.98	0.46
1:C:347:GLU:HA	1:C:434:LYS:HD3	1.97	0.46
1:A:314:PHE:HB3	1:C:314:PHE:CZ	2.51	0.46
1:A:439:TYR:HD1	1:A:440:ILE:N	2.14	0.46
1:A:634:LYS:HE3	1:A:695:TYR:CD2	2.51	0.46
1:D:383:TYR:CD2	1:D:718:ILE:HD11	2.50	0.46
1:D:603:VAL:O	1:D:603:VAL:HG13	2.15	0.46
1:D:680:LEU:HD23	1:D:680:LEU:HA	1.75	0.46
1:B:329:ILE:CG2	1:B:330:VAL:N	2.78	0.45
1:A:464:THR:HG22	1:B:464:THR:HG22	1.98	0.45
1:A:542:MET:HE1	1:A:612:LEU:CB	2.42	0.45
1:B:346:LYS:HE2	1:C:332:ARG:HH22	1.80	0.45
1:B:697:ARG:HD3	1:B:698:PHE:CE2	2.51	0.45
1:B:353:LYS:HA	1:B:718:ILE:HD12	1.99	0.45
1:B:531:HIS:O	1:B:531:HIS:CD2	2.69	0.45
1:C:696:ASP:HA	1:C:700:SER:HB3	1.98	0.45
1:A:380:TYR:CE1	1:A:715:HIS:ND1	2.85	0.45
1:B:338:ARG:O	1:B:341:TYR:HB3	2.16	0.45
1:B:554:SER:C	1:B:556:GLY:H	2.20	0.45
1:C:434:LYS:C	1:C:436:ASN:H	2.20	0.45
1:D:444:HIS:O	1:D:511:ARG:NH1	2.49	0.45
1:A:572:GLU:O	1:A:678:LYS:HE2	2.17	0.45
1:D:451:LEU:HD12	1:D:451:LEU:N	2.26	0.45
1:A:507:ILE:HG21	1:A:709:TYR:CD2	2.52	0.45
1:D:459:ARG:HG3	1:D:459:ARG:O	2.17	0.45
1:A:367:ASP:O	1:A:370:LYS:HB3	2.16	0.45
1:D:366:SER:HA	1:D:370:LYS:HD2	1.99	0.45
1:D:663:PRO:HG3	1:D:694:PHE:CD1	2.50	0.45
1:A:648:ASP:O	1:A:649:LYS:HB2	2.17	0.45
1:A:652:ARG:C	1:A:654:PHE:N	2.67	0.45
1:B:355:ILE:HG22	1:B:357:PHE:CE2	2.52	0.45
1:A:484:SER:HA	1:A:485:PRO:HD3	1.78	0.45
1:B:548:ARG:NH2	1:B:622:ASP:OD1	2.36	0.45
1:C:367:ASP:OD2	1:C:511:ARG:HD3	2.17	0.45
1:C:572:GLU:OE1	1:C:678:LYS:HE3	2.16	0.45
1:A:577:TYR:OH	1:A:680:LEU:HG	2.17	0.44
1:C:665:PRO:HG3	1:C:687:TYR:CZ	2.53	0.44
1:C:662:LEU:HB2	1:C:663:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:HIS:NE2	1:D:329:ILE:HD13	2.31	0.44
1:D:441:GLN:O	1:D:482:LEU:HA	2.18	0.44
1:B:343:LEU:HD22	1:D:314:PHE:HE1	1.83	0.44
1:C:559:LEU:HD23	1:C:587:ILE:HG23	2.00	0.44
1:C:647:TYR:O	1:C:648:ASP:HB2	2.17	0.44
1:D:677:LEU:HD12	1:D:677:LEU:HA	1.82	0.44
1:A:670:PRO:HD2	1:A:671:TYR:CE2	2.52	0.44
1:D:325:HIS:CE1	1:D:329:ILE:CD1	3.01	0.44
1:D:460:MET:HA	1:D:461:PRO:HD2	1.87	0.44
1:C:639:PHE:HZ	1:C:663:PRO:HD2	1.81	0.44
1:D:621:THR:HG23	1:D:622:ASP:N	2.32	0.44
1:C:406:ARG:O	1:C:407:ASN:HB2	2.18	0.44
1:C:701:VAL:HG12	1:C:701:VAL:O	2.17	0.44
1:A:525:LEU:O	1:A:529:ARG:HG3	2.17	0.44
1:B:510:PRO:HB3	1:B:707:SER:OG	2.17	0.44
1:C:315:LYS:HE3	1:C:315:LYS:HB2	1.88	0.44
1:A:325:HIS:CE1	1:A:329:ILE:CD1	3.01	0.44
1:B:325:HIS:CE1	1:B:340:LEU:HB2	2.53	0.44
1:C:483:ILE:CG2	1:C:484:SER:N	2.80	0.44
1:C:606:TYR:CD1	1:C:612:LEU:HD21	2.53	0.44
1:D:633:LEU:HB3	1:D:635:ARG:HD3	2.00	0.44
1:B:350:VAL:HA	1:B:417:GLU:O	2.18	0.43
1:C:418:ALA:O	1:C:437:GLN:HG2	2.17	0.43
1:D:586:LEU:HD23	1:D:586:LEU:HA	1.84	0.43
1:D:647:TYR:O	1:D:648:ASP:HB2	2.17	0.43
1:A:528:ILE:HG22	1:A:615:ILE:HD13	2.00	0.43
1:D:669:GLU:HG2	1:D:671:TYR:H	1.83	0.43
1:B:528:ILE:HD11	1:B:611:GLU:HG2	1.99	0.43
1:B:638:PHE:HZ	1:B:683:VAL:HG21	1.82	0.43
1:A:356:VAL:HG23	1:A:418:ALA:CB	2.46	0.43
1:A:559:LEU:CD1	1:A:559:LEU:C	2.86	0.43
1:C:559:LEU:HD12	1:C:559:LEU:O	2.18	0.43
1:C:375:TYR:CZ	1:C:708:GLN:HA	2.53	0.43
1:C:450:ARG:HA	1:C:655:TYR:CE2	2.53	0.43
1:D:386:ILE:HG21	1:D:414:ALA:HB1	1.99	0.43
1:D:559:LEU:HD23	1:D:587:ILE:HG23	1.99	0.43
1:A:426:ARG:HG2	1:A:475:GLU:HG2	2.01	0.43
1:B:607:ASN:OD1	1:B:607:ASN:N	2.51	0.43
1:C:662:LEU:HB2	1:C:663:PRO:CD	2.47	0.43
1:D:566:LEU:HD23	1:D:566:LEU:HA	1.69	0.43
1:D:712:ASP:O	1:D:713:LEU:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:TYR:CE1	1:B:401:ALA:HB2	2.54	0.43
1:A:581:LEU:O	1:A:603:VAL:HG12	2.19	0.43
1:B:487:ARG:HA	1:B:487:ARG:HD3	1.78	0.43
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.92	0.43
1:C:525:LEU:O	1:C:529:ARG:HG3	2.19	0.43
1:A:439:TYR:CD1	1:A:439:TYR:C	2.89	0.42
1:B:697:ARG:HD3	1:B:698:PHE:CZ	2.54	0.42
1:C:677:LEU:HD12	1:C:677:LEU:HA	1.83	0.42
1:A:552:PHE:O	1:A:553:VAL:HG13	2.19	0.42
1:C:470:ARG:NH1	1:C:470:ARG:CG	2.68	0.42
1:D:327:LYS:HZ3	4:D:735:EDT:C6	2.32	0.42
1:D:648:ASP:HB2	1:D:651:LEU:HB3	2.01	0.42
1:B:351:LYS:HD2	1:B:417:GLU:OE1	2.19	0.42
1:D:325:HIS:CE1	1:D:329:ILE:HD13	2.54	0.42
1:B:648:ASP:HB2	1:B:651:LEU:CB	2.43	0.42
1:A:375:TYR:CZ	1:A:708:GLN:HA	2.55	0.42
1:B:493:PHE:O	1:B:497:PHE:HB2	2.19	0.42
1:C:718:ILE:HG13	1:C:718:ILE:O	2.19	0.42
1:D:458:VAL:HG12	1:D:460:MET:HB2	2.01	0.42
1:B:405:LYS:O	1:B:411:TYR:HB2	2.19	0.42
1:C:559:LEU:HD13	1:C:560:PHE:C	2.40	0.42
1:C:687:TYR:O	1:C:691:ILE:HG13	2.19	0.42
1:A:542:MET:HE3	1:A:616:SER:OG	2.19	0.42
1:A:670:PRO:HD2	1:A:671:TYR:CD2	2.54	0.42
1:C:353:LYS:HG2	3:C:732:CL:CL	2.57	0.42
1:D:346:LYS:O	1:D:349:ASN:HB2	2.20	0.42
1:D:488:TYR:OH	1:D:655:TYR:HB2	2.19	0.42
1:C:433:LYS:HE2	1:C:433:LYS:O	2.20	0.42
4:D:735:EDT:O15	4:D:735:EDT:H071	2.18	0.42
1:A:546:THR:HG23	1:A:624:SER:HB2	2.01	0.41
1:B:614:LEU:O	1:B:635:ARG:NH1	2.53	0.41
1:C:329:ILE:HG22	1:C:330:VAL:N	2.34	0.41
1:C:662:LEU:H	1:C:662:LEU:HD22	1.81	0.41
1:D:559:LEU:HD13	1:D:560:PHE:O	2.20	0.41
1:A:352:PRO:O	1:A:718:ILE:HD12	2.20	0.41
1:A:714:ILE:O	1:A:718:ILE:CG2	2.63	0.41
1:B:403:LYS:CE	3:B:736:CL:CL	3.03	0.41
1:B:443:TRP:HB3	5:B:739:HOH:O	2.20	0.41
1:D:385:TYR:O	1:D:401:ALA:HA	2.20	0.41
1:A:658:TYR:C	1:A:660:GLU:H	2.24	0.41
4:A:738:EDT:H072	4:A:738:EDT:H022	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:ARG:HD3	1:C:698:PHE:CZ	2.55	0.41
1:D:349:ASN:HD22	1:D:349:ASN:HA	1.65	0.41
1:C:325:HIS:CE1	1:C:329:ILE:HD13	2.55	0.41
1:C:470:ARG:NH1	1:C:471:ASN:OD1	2.53	0.41
1:C:718:ILE:O	1:C:718:ILE:CG1	2.68	0.41
1:D:458:VAL:HG13	1:D:460:MET:HE2	2.02	0.41
1:D:380:TYR:CE1	1:D:715:HIS:CG	3.09	0.41
1:D:420:HIS:CE1	1:D:718:ILE:HG22	2.55	0.41
1:D:632:ILE:HG12	1:D:699:CYS:HB3	2.02	0.41
1:A:376:MET:HB3	1:A:385:TYR:OH	2.20	0.41
1:B:431:LEU:HA	1:B:431:LEU:HD23	1.85	0.41
1:D:347:GLU:HA	1:D:434:LYS:HD3	2.02	0.41
1:D:456:LYS:HA	1:D:456:LYS:CE	2.48	0.41
1:D:581:LEU:O	1:D:603:VAL:HG12	2.20	0.41
1:A:492:ILE:HD13	1:A:655:TYR:CG	2.56	0.41
4:A:738:EDT:C10	4:A:738:EDT:H062	2.51	0.41
1:C:450:ARG:HD2	1:C:653:GLY:HA2	2.03	0.41
1:C:523:GLU:O	1:C:523:GLU:HG2	2.20	0.41
1:A:352:PRO:HA	1:A:419:SER:HB3	2.02	0.41
1:A:485:PRO:HB2	1:A:486:ASN:ND2	2.36	0.41
1:A:662:LEU:CD2	1:A:662:LEU:N	2.84	0.41
1:B:450:ARG:HA	1:B:655:TYR:CE2	2.56	0.41
1:B:600:ALA:C	1:B:601:ILE:HD13	2.41	0.41
1:C:448:LEU:HD13	1:C:627:MET:HE1	2.02	0.41
1:C:581:LEU:O	1:C:603:VAL:HG12	2.21	0.41
1:D:397:VAL:HG12	1:D:398:PRO:O	2.21	0.41
1:D:434:LYS:C	1:D:436:ASN:H	2.24	0.41
1:D:484:SER:HA	1:D:485:PRO:HD3	1.75	0.41
1:A:559:LEU:HD22	1:A:560:PHE:O	2.21	0.41
1:C:483:ILE:HD11	1:C:710:ILE:HG13	2.02	0.41
1:C:705:LYS:O	1:C:708:GLN:HB3	2.21	0.41
1:C:562:LEU:H	1:C:562:LEU:HG	1.61	0.40
1:D:347:GLU:C	1:D:349:ASN:H	2.25	0.40
1:D:531:HIS:CD2	1:D:531:HIS:O	2.75	0.40
1:A:603:VAL:HG22	1:A:603:VAL:O	2.21	0.40
1:C:352:PRO:HA	1:C:419:SER:HB3	2.04	0.40
1:D:591:LEU:HD23	1:D:591:LEU:HA	1.96	0.40
1:A:669:GLU:HG2	1:A:671:TYR:H	1.86	0.40
1:A:388:SER:HA	1:A:404:VAL:HG23	2.03	0.40
1:B:680:LEU:HD23	1:B:680:LEU:HA	1.84	0.40
1:B:687:TYR:C	1:B:689:GLU:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:PRO:HD2	1:C:489:SER:HB2	2.04	0.40
1:D:620:ILE:HD11	1:D:677:LEU:HD21	2.04	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	403/729 (55%)	369 (92%)	33 (8%)	1 (0%)	47 75
1	B	409/729 (56%)	366 (90%)	40 (10%)	3 (1%)	22 50
1	C	409/729 (56%)	363 (89%)	41 (10%)	5 (1%)	13 35
1	D	410/729 (56%)	372 (91%)	37 (9%)	1 (0%)	47 75
All	All	1631/2916 (56%)	1470 (90%)	151 (9%)	10 (1%)	25 53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	550	ASP
1	C	535	PRO
1	D	649	LYS
1	A	689	GLU
1	B	443	TRP
1	B	550	ASP
1	C	565	ASP
1	B	555	LYS
1	C	443	TRP
1	C	714	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/674 (56%)	332 (88%)	44 (12%)	5	14
1	B	378/674 (56%)	331 (88%)	47 (12%)	4	12
1	C	378/674 (56%)	341 (90%)	37 (10%)	8	21
1	D	379/674 (56%)	339 (89%)	40 (11%)	6	18
All	All	1511/2696 (56%)	1343 (89%)	168 (11%)	6	16

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	LEU
1	A	329	ILE
1	A	332	ARG
1	A	333	ARG
1	A	346	LYS
1	A	359	SER
1	A	367	ASP
1	A	403	LYS
1	A	433	LYS
1	A	435	GLU
1	A	439	TYR
1	A	450	ARG
1	A	451	LEU
1	A	456	LYS
1	A	460	MET
1	A	463	THR
1	A	472	PHE
1	A	486	ASN
1	A	487	ARG
1	A	491	GLU
1	A	511	ARG
1	A	537	ASP
1	A	549	ASP
1	A	553	VAL

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Mol	Chain	Res	Type
1	A	559	LEU
1	A	578	VAL
1	A	585	TYR
1	A	589	ASN
1	A	597	GLU
1	A	607	ASN
1	A	619	LEU
1	A	622	ASP
1	A	625	SER
1	A	635	ARG
1	A	656	MET
1	A	660	GLU
1	A	662	LEU
1	A	669	GLU
1	A	673	LEU
1	A	676	GLU
1	A	677	LEU
1	A	678	LYS
1	A	718	ILE
1	A	722	LEU
1	B	316	VAL
1	B	323	LEU
1	B	329	ILE
1	B	333	ARG
1	B	343	LEU
1	B	347	GLU
1	B	367	ASP
1	B	382	ASN
1	B	402	GLU
1	B	407	ASN
1	B	439	TYR
1	B	450	ARG
1	B	451	LEU
1	B	456	LYS
1	B	464	THR
1	B	465	THR
1	B	470	ARG
1	B	472	PHE
1	B	486	ASN
1	B	487	ARG
1	B	491	GLU
1	B	514	VAL

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Mol	Chain	Res	Type
1	B	546	THR
1	B	548	ARG
1	B	555	LYS
1	B	559	LEU
1	B	578	VAL
1	B	583	MET
1	B	585	TYR
1	B	597	GLU
1	B	603	VAL
1	B	604	SER
1	B	609	VAL
1	B	622	ASP
1	B	623	TYR
1	B	635	ARG
1	B	656	MET
1	B	660	GLU
1	B	662	LEU
1	B	669	GLU
1	B	673	LEU
1	B	676	GLU
1	B	678	LYS
1	B	703	ASN
1	B	718	ILE
1	B	720	GLU
1	B	722	LEU
1	C	315	LYS
1	C	323	LEU
1	C	329	ILE
1	C	333	ARG
1	C	388	SER
1	C	403	LYS
1	C	406	ARG
1	C	439	TYR
1	C	450	ARG
1	C	451	LEU
1	C	456	LYS
1	C	460	MET
1	C	470	ARG
1	C	472	PHE
1	C	487	ARG
1	C	491	GLU
1	C	536	SER

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Mol	Chain	Res	Type
1	C	553	VAL
1	C	559	LEU
1	C	567	ASP
1	C	585	TYR
1	C	594	SER
1	C	597	GLU
1	C	604	SER
1	C	622	ASP
1	C	623	TYR
1	C	625	SER
1	C	656	MET
1	C	660	GLU
1	C	662	LEU
1	C	668	THR
1	C	669	GLU
1	C	673	LEU
1	C	677	LEU
1	C	678	LYS
1	C	718	ILE
1	C	722	LEU
1	D	316	VAL
1	D	323	LEU
1	D	329	ILE
1	D	333	ARG
1	D	343	LEU
1	D	346	LYS
1	D	356	VAL
1	D	403	LYS
1	D	439	TYR
1	D	450	ARG
1	D	451	LEU
1	D	456	LYS
1	D	460	MET
1	D	464	THR
1	D	470	ARG
1	D	472	PHE
1	D	487	ARG
1	D	491	GLU
1	D	511	ARG
1	D	549	ASP
1	D	559	LEU
1	D	585	TYR

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Mol	Chain	Res	Type
1	D	594	SER
1	D	597	GLU
1	D	619	LEU
1	D	622	ASP
1	D	623	TYR
1	D	625	SER
1	D	647	TYR
1	D	656	MET
1	D	660	GLU
1	D	662	LEU
1	D	669	GLU
1	D	673	LEU
1	D	676	GLU
1	D	677	LEU
1	D	702	ASP
1	D	718	ILE
1	D	720	GLU
1	D	722	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	531	HIS
1	B	349	ASN
1	B	531	HIS
1	B	679	ASN
1	B	686	GLN
1	B	703	ASN
1	B	708	GLN
1	C	349	ASN
1	C	531	HIS
1	C	686	GLN
1	D	349	ASN
1	D	531	HIS
1	D	568	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 18 are monoatomic - leaving 10 for Mogul analysis.

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	730	-	4,4,4	0.82	0	6,6,6	0.65	0
2	PO4	C	731	-	4,4,4	0.85	0	6,6,6	0.47	0
4	EDT	A	738	-	19,19,19	1.59	4 (21%)	24,24,24	1.01	1 (4%)
2	PO4	A	731	-	4,4,4	0.82	0	6,6,6	0.47	0
2	PO4	B	731	-	4,4,4	0.89	0	6,6,6	0.58	0
4	EDT	D	735	-	19,19,19	1.62	4 (21%)	24,24,24	1.31	3 (12%)
2	PO4	D	730	-	4,4,4	0.96	0	6,6,6	0.33	0
2	PO4	D	731	-	4,4,4	0.72	0	6,6,6	0.75	0
2	PO4	C	730	-	4,4,4	0.83	0	6,6,6	0.49	0
2	PO4	B	730	-	4,4,4	0.88	0	6,6,6	0.41	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
4	EDT	A	738	-	-	14/21/21/21	-
4	EDT	D	735	-	-	13/21/21/21	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	735	EDT	O16-C10	3.32	1.41	1.30
4	A	738	EDT	O16-C10	3.10	1.41	1.30
4	D	735	EDT	O17-C1	3.09	1.41	1.30
4	D	735	EDT	O14-C12	2.99	1.40	1.30
4	A	738	EDT	O14-C12	2.98	1.40	1.30
4	A	738	EDT	O17-C1	2.98	1.40	1.30
4	A	738	EDT	O20-C5	2.93	1.40	1.30
4	D	735	EDT	O20-C5	2.90	1.40	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	735	EDT	C2-N3-C4	3.19	118.75	111.54
4	D	735	EDT	O20-C5-O19	-2.37	117.39	123.30
4	A	738	EDT	O14-C12-O13	-2.02	118.28	123.30
4	D	735	EDT	C4-N3-C6	2.01	116.84	111.94

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	738	EDT	N3-C4-C5-O19
4	A	738	EDT	C5-C4-N3-C6
4	A	738	EDT	C7-C6-N3-C2
4	A	738	EDT	C10-C9-N8-C7
4	A	738	EDT	N8-C11-C12-O13
4	A	738	EDT	N8-C11-C12-O14
4	D	735	EDT	N3-C4-C5-O20
4	D	735	EDT	O18-C1-C2-N3
4	D	735	EDT	C10-C9-N8-C7
4	D	735	EDT	C12-C11-N8-C9
4	D	735	EDT	O16-C10-C9-N8
4	D	735	EDT	O15-C10-C9-N8
4	D	735	EDT	N8-C11-C12-O13
4	D	735	EDT	N8-C11-C12-O14
4	A	738	EDT	N3-C4-C5-O20
4	A	738	EDT	O16-C10-C9-N8
4	A	738	EDT	O15-C10-C9-N8
4	A	738	EDT	N3-C6-C7-N8
4	D	735	EDT	C5-C4-N3-C6
4	D	735	EDT	C1-C2-N3-C4
4	A	738	EDT	C7-C6-N3-C4

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Mol	Chain	Res	Type	Atoms
4	A	738	EDT	C6-C7-N8-C9
4	D	735	EDT	N3-C4-C5-O19
4	D	735	EDT	C12-C11-N8-C7
4	D	735	EDT	C10-C9-N8-C11
4	A	738	EDT	C5-C4-N3-C2
4	A	738	EDT	C12-C11-N8-C7

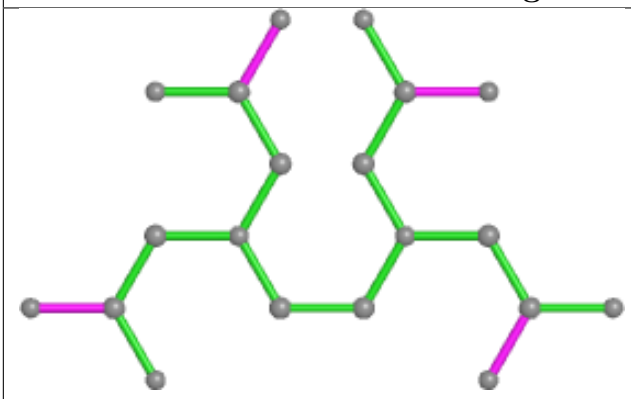
There are no ring outliers.

5 monomers are involved in 20 short contacts:

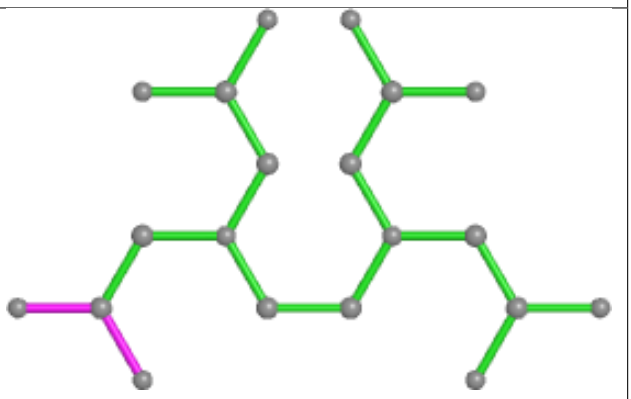
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	738	EDT	10	0
2	A	731	PO4	1	0
2	B	731	PO4	1	0
4	D	735	EDT	7	0
2	D	731	PO4	1	0

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 then 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.

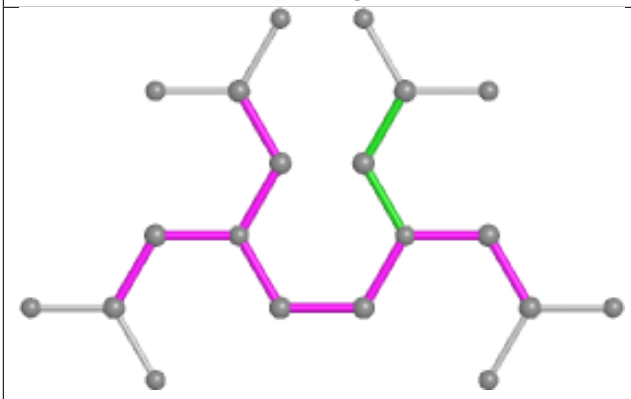
Ligand EDT A 738



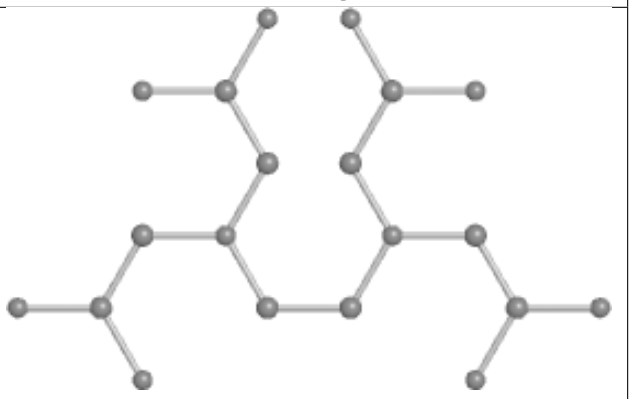
Bond lengths



Bond angles

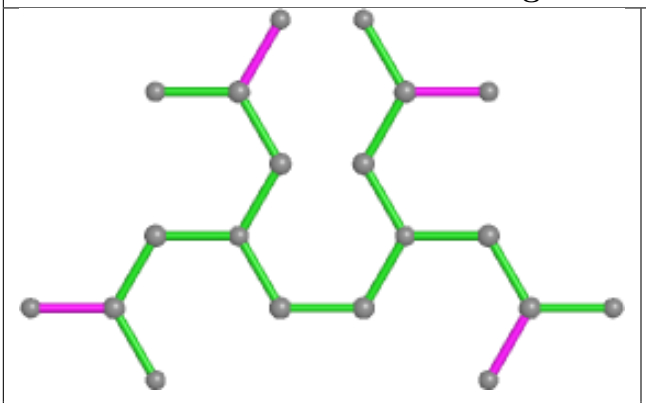


Torsions

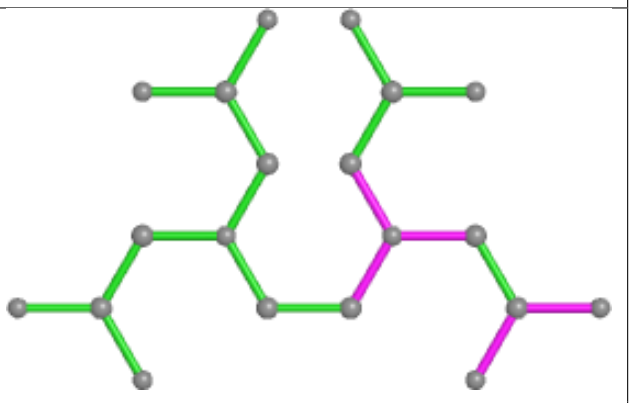


Rings

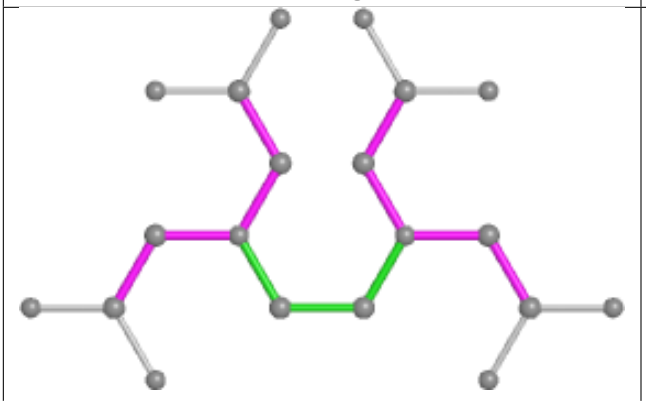
Ligand EDT D 735



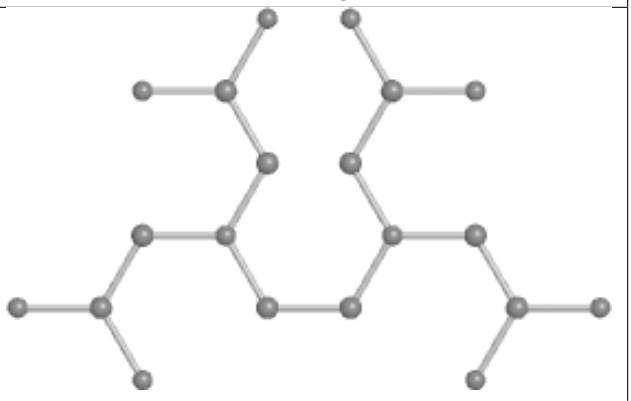
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	407/729 (55%)	-0.19	11 (2%)	54	50	57, 87, 151, 221	0
1	B	411/729 (56%)	-0.20	16 (3%)	39	34	58, 84, 147, 265	0
1	C	411/729 (56%)	-0.06	19 (4%)	32	27	59, 96, 163, 264	0
1	D	412/729 (56%)	-0.11	19 (4%)	32	27	63, 89, 163, 306	0
All	All	1641/2916 (56%)	-0.14	65 (3%)	38	32	57, 89, 160, 306	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	724	HIS	7.9
1	C	558	TYR	7.3
1	D	652	ARG	5.9
1	B	555	LYS	5.6
1	D	558	TYR	5.1
1	C	557	LYS	5.1
1	B	557	LYS	5.1
1	C	556	GLY	5.0
1	A	555	LYS	4.8
1	B	558	TYR	4.7
1	D	556	GLY	4.7
1	C	313	ALA	4.5
1	C	652	ARG	4.5
1	B	652	ARG	4.5
1	D	649	LYS	4.4
1	B	649	LYS	4.3
1	C	457	VAL	4.2
1	A	459	ARG	4.2
1	A	649	LYS	3.9
1	C	649	LYS	3.9
1	C	555	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	459	ARG	3.8
1	D	557	LYS	3.7
1	A	554	SER	3.6
1	B	560	PHE	3.6
1	A	458	VAL	3.5
1	D	554	SER	3.5
1	C	723	GLU	3.5
1	B	556	GLY	3.4
1	C	463	THR	3.4
1	A	585	TYR	3.3
1	D	555	LYS	3.2
1	B	554	SER	3.1
1	A	652	ARG	3.1
1	C	459	ARG	3.1
1	B	650	GLY	2.9
1	B	457	VAL	2.9
1	A	560	PHE	2.9
1	C	559	LEU	2.9
1	C	553	VAL	2.9
1	D	650	GLY	2.8
1	C	552	PHE	2.6
1	A	463	THR	2.6
1	C	650	GLY	2.6
1	D	550	ASP	2.5
1	A	723	GLU	2.5
1	D	463	THR	2.5
1	D	462	GLY	2.5
1	B	460	MET	2.5
1	C	456	LYS	2.5
1	C	458	VAL	2.5
1	D	313	ALA	2.4
1	D	723	GLU	2.3
1	C	554	SER	2.3
1	D	552	PHE	2.3
1	A	552	PHE	2.2
1	D	553	VAL	2.2
1	B	537	ASP	2.2
1	D	457	VAL	2.2
1	D	585	TYR	2.2
1	B	356	VAL	2.1
1	B	561	GLU	2.1
1	C	460	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	348	ASP	2.1
1	B	458	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 monosaccharides 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, 95^{th} 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	CL	A	736	1/1	0.61	0.44	111,111,111,111	0
3	CL	B	734	1/1	0.68	0.51	141,141,141,141	0
3	CL	D	733	1/1	0.69	0.34	124,124,124,124	0
3	CL	A	735	1/1	0.71	0.66	104,104,104,104	0
3	CL	A	737	1/1	0.77	0.22	115,115,115,115	0
4	EDT	A	738	20/20	0.78	0.30	134,134,134,134	0
4	EDT	D	735	20/20	0.78	0.29	132,132,132,132	0
3	CL	B	733	1/1	0.80	0.48	109,109,109,109	0
3	CL	C	733	1/1	0.83	0.27	108,108,108,108	0
3	CL	D	732	1/1	0.85	0.11	107,107,107,107	0
3	CL	B	737	1/1	0.87	0.21	99,99,99,99	0
3	CL	C	732	1/1	0.88	0.20	119,119,119,119	0
3	CL	A	732	1/1	0.88	0.57	126,126,126,126	0
3	CL	B	735	1/1	0.89	0.18	107,107,107,107	0
3	CL	D	736	1/1	0.89	0.18	87,87,87,87	0
2	PO4	C	731	5/5	0.90	0.26	152,152,152,152	0
3	CL	D	734	1/1	0.92	0.43	113,113,113,113	0
2	PO4	D	731	5/5	0.93	0.15	133,133,133,133	0
3	CL	B	736	1/1	0.94	0.50	140,140,140,140	0
2	PO4	B	731	5/5	0.95	0.17	123,123,123,123	0
3	CL	A	734	1/1	0.95	0.16	102,102,102,102	0

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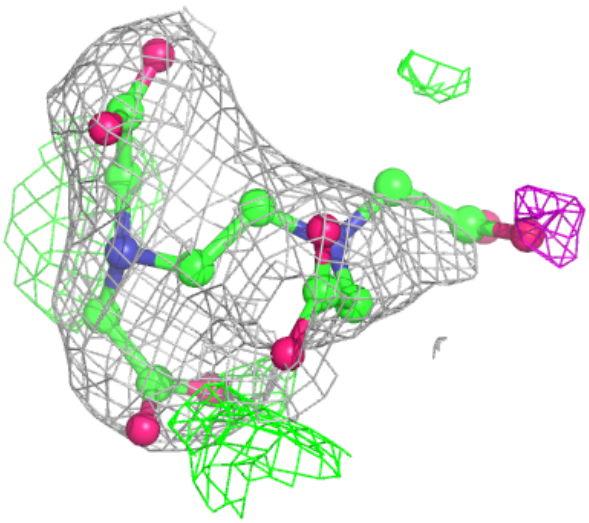
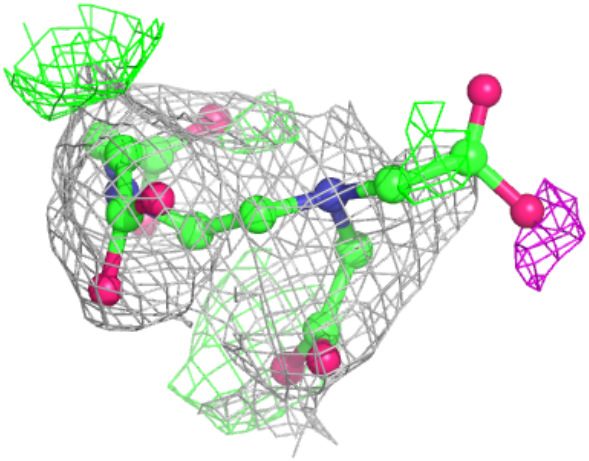
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	C	730	5/5	0.95	0.10	125,125,125,125	0
2	PO4	A	731	5/5	0.96	0.12	124,124,124,124	0
2	PO4	B	730	5/5	0.97	0.10	112,112,112,112	0
3	CL	A	733	1/1	0.98	0.39	93,93,93,93	0
2	PO4	A	730	5/5	0.98	0.09	102,102,102,102	0
2	PO4	D	730	5/5	0.98	0.12	125,125,125,125	0
3	CL	B	732	1/1	0.99	0.07	69,69,69,69	0

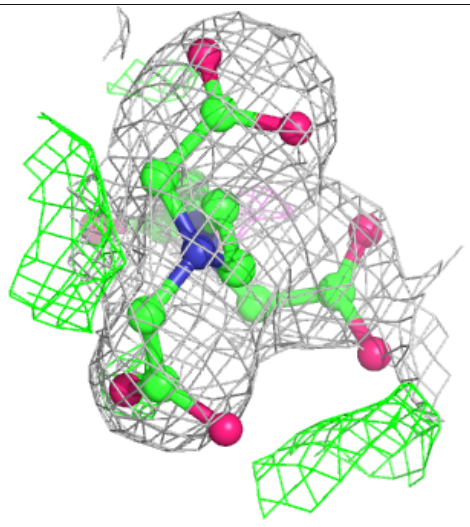
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDT A 738:

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

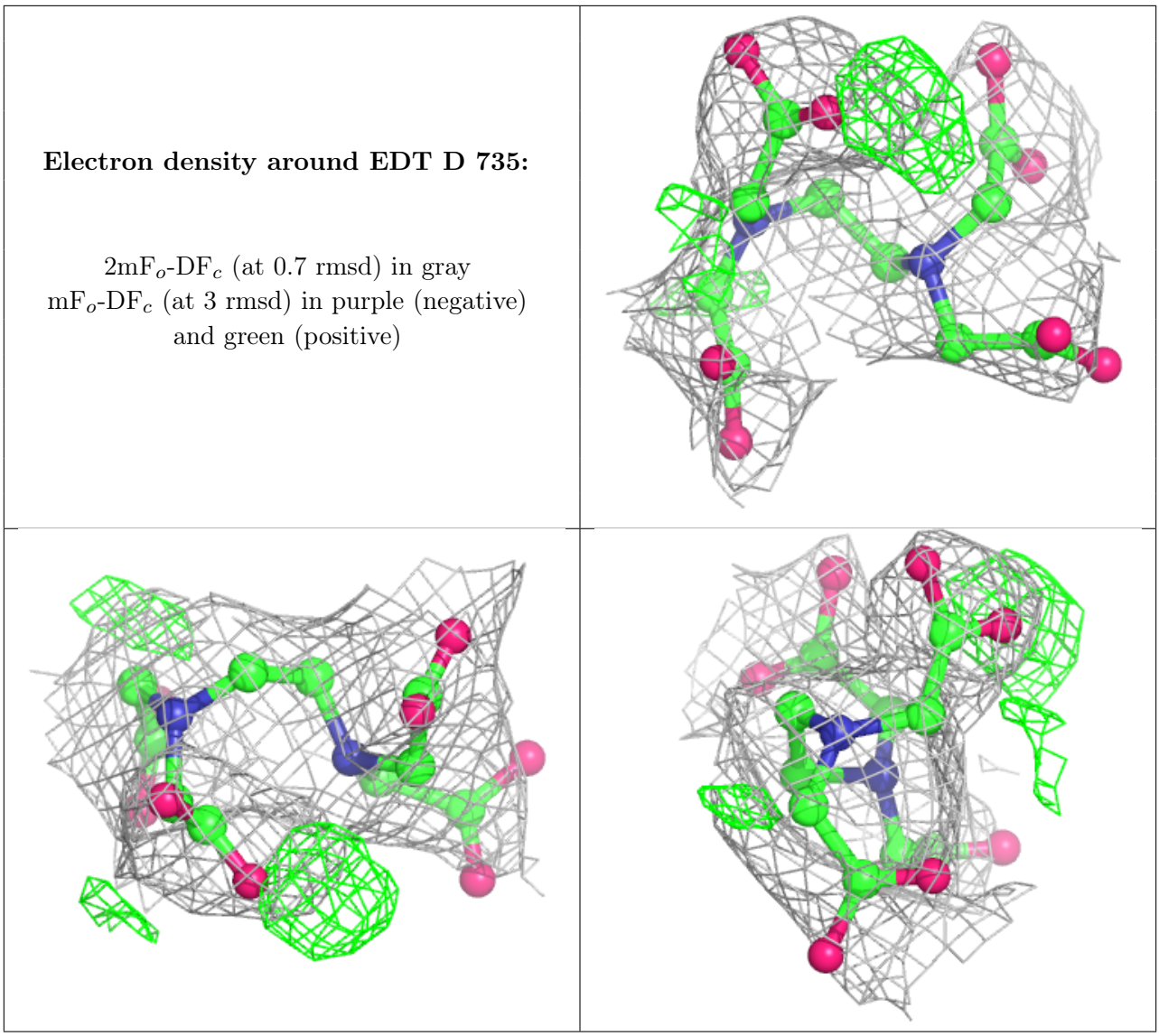






Electron density around EDT D 735:

$2mF_o$-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

There are no such residues in this entry.