



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 02:18 PM EDT

PDB ID : 3L7K
Title : Structure of the Wall Teichoic Acid Polymerase TagF, H444N + CDPG (15 minute soak)
Authors : Strynadka, N.C.J.; Lovering, A.L.
Deposited on : 2009-12-28
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2
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) : 2.23.2

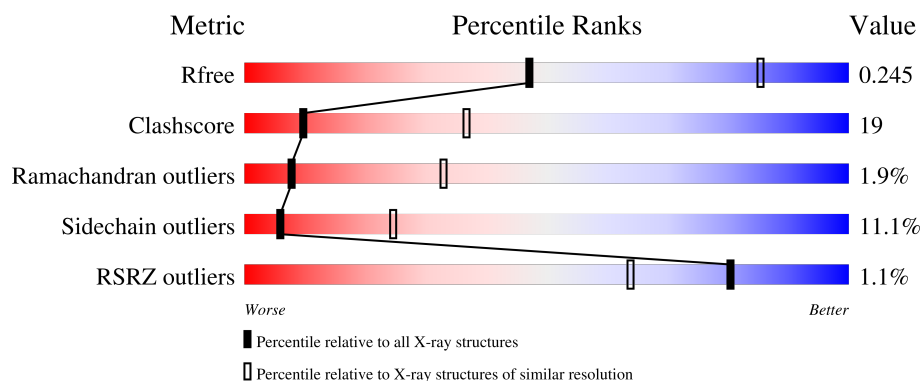
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	729	<div> <div></div> <div>34%20%•44%</div> </div>
1	B	729	<div> <div>%</div> <div>34%18%•44%</div> </div>
1	C	729	<div> <div>%</div> <div>30%22%•44%</div> </div>
1	D	729	<div> <div>%</div> <div>30%21%•46%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	730	-	-	X	-
3	CL	C	734	-	-	-	X
4	EDT	A	739	-	-	X	X
4	EDT	D	735	-	-	X	X
6	EDO	D	734	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13843 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	410	Total	C	N	O	S	0	0	0
			3462	2224	577	650	11			
1	B	409	Total	C	N	O	S	0	0	0
			3446	2212	575	648	11			
1	C	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	D	395	Total	C	N	O	S	0	0	0
			3334	2140	558	625	11			

There are 36 discrepancies between the modelled and reference sequences:

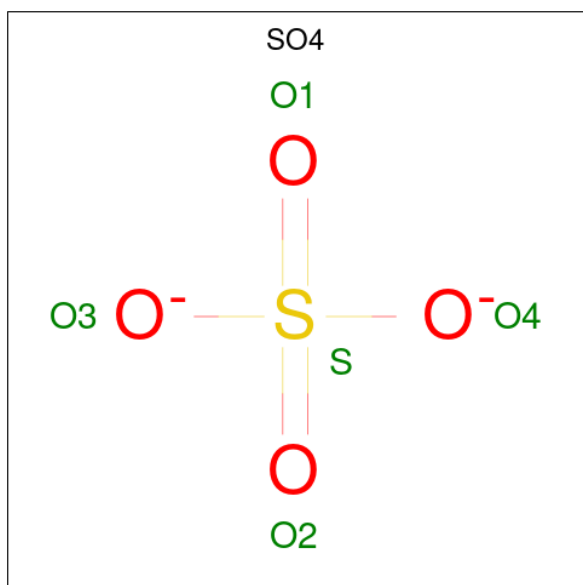
Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASN	HIS	engineered mutation	UNP Q5HLM5
A	722	LEU	-	expression tag	UNP Q5HLM5
A	723	GLU	-	expression tag	UNP Q5HLM5
A	724	HIS	-	expression tag	UNP Q5HLM5
A	725	HIS	-	expression tag	UNP Q5HLM5
A	726	HIS	-	expression tag	UNP Q5HLM5
A	727	HIS	-	expression tag	UNP Q5HLM5
A	728	HIS	-	expression tag	UNP Q5HLM5
A	729	HIS	-	expression tag	UNP Q5HLM5
B	444	ASN	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	444	ASN	HIS	engineered mutation	UNP Q5HLM5
C	722	LEU	-	expression tag	UNP Q5HLM5
C	723	GLU	-	expression tag	UNP Q5HLM5

Continued on next page...

Continued from previous page...

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	444	ASN	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

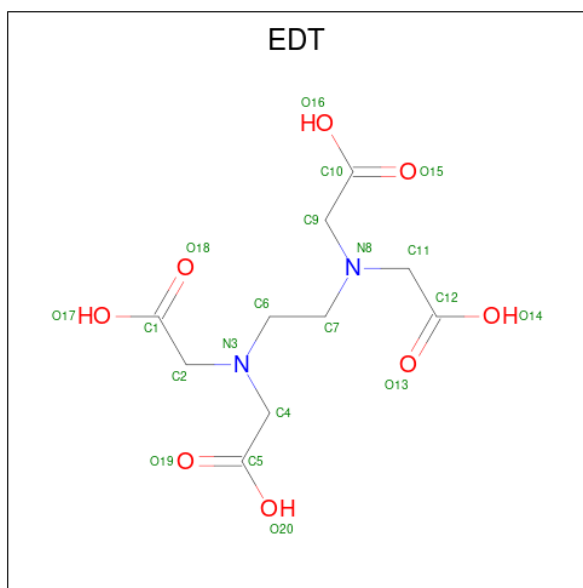
Continued from previous page...

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

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

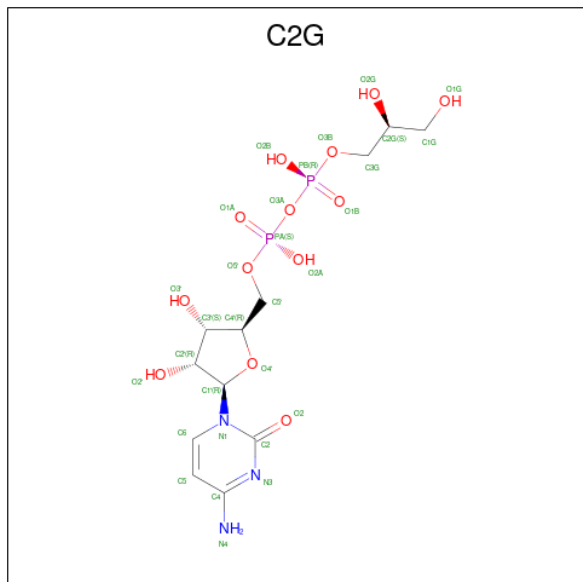
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	Cl	0	0
			9	9		
3	B	6	Total	Cl	0	0
			6	6		
3	C	5	Total	Cl	0	0
			5	5		
3	D	2	Total	Cl	0	0
			2	2		

- Molecule 4 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: C₁₀H₁₆N₂O₈).



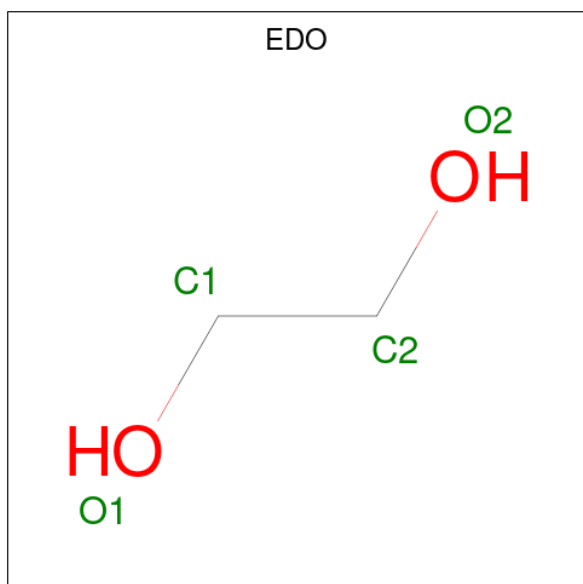
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	10	2	8		
4	D	1	Total	C	N	O	0	0
			20	10	2	8		

- Molecule 5 is [CYTIDINE-5'-PHOSPHATE] GLYCERYLPHOSPHORIC ACID ESTER (three-letter code: C2G) (formula: $C_{12}H_{21}N_3O_{13}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	D	1	30	12	3	13	2	0	0

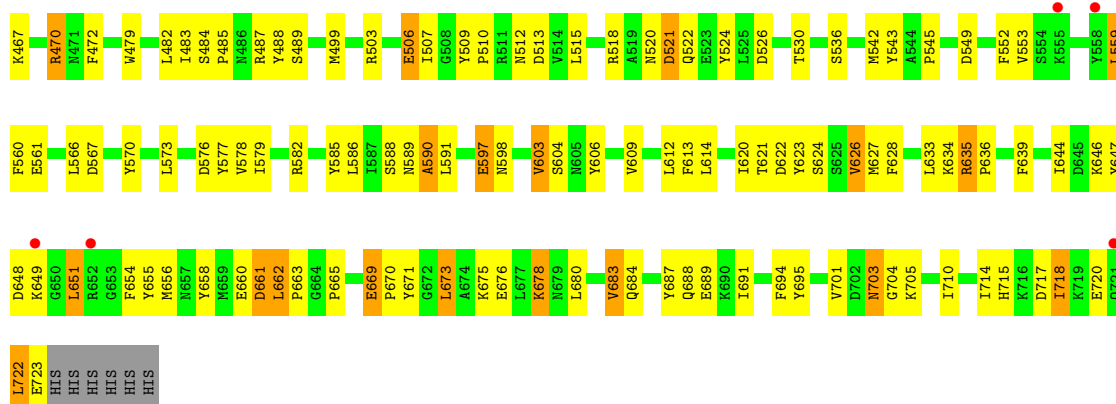
- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



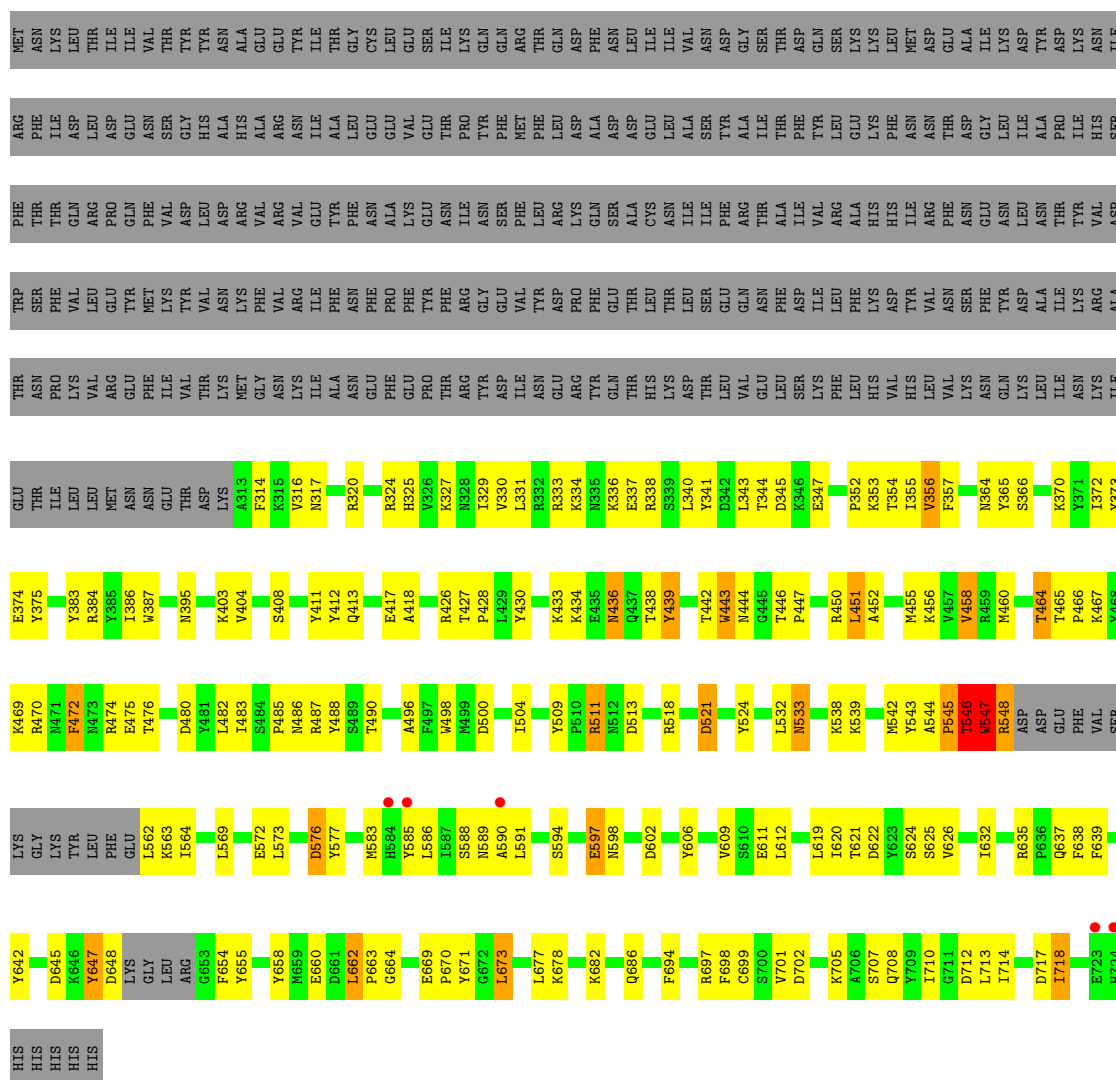
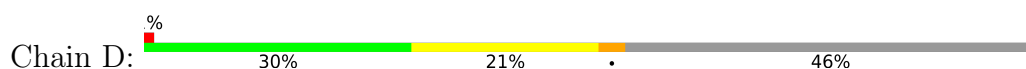
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	D	1	4	2	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	O 1	0	0
7	B	3	Total 3	O 3	0	0
7	C	2	Total 2	O 2	0	0
7	D	2	Total 2	O 2	0	0



• Molecule 1: Teichoic acid biosynthesis protein F



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	222.04Å 222.04Å 100.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 3.10 19.86 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.86-3.10) 99.3 (19.86-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.09Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.190 , 0.252 0.184 , 0.245	Depositor DCC
R_{free} test set	2285 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	87.2	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13843	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, EDT, C2G, CL, SO4

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	0.44	0/3551	0.59	0/4798
1	B	0.43	0/3533	0.58	1/4773 (0.0%)
1	C	0.40	0/3556	0.58	0/4805
1	D	0.43	0/3419	0.59	1/4621 (0.0%)
All	All	0.42	0/14059	0.59	2/18997 (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	D	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	547	TRP	N-CA-C	5.62	126.18	111.00
1	B	662	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	546	THR	Peptide
1	D	585	TYR	Peptide

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	3462	0	3369	120	0
1	B	3446	0	3351	121	0
1	C	3467	0	3374	146	0
1	D	3334	0	3238	146	0
2	A	15	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	9	0	0	3	0
3	B	6	0	0	3	0
3	C	5	0	0	1	0
3	D	2	0	0	1	0
4	A	20	0	16	11	0
4	D	20	0	16	8	0
5	D	30	0	19	2	0
6	D	4	0	6	4	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	13843	0	13389	525	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 19.

All (525) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:MET:HE1	1:B:612:LEU:HB3	1.33	1.05
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.17	1.03
1:A:324:ARG:HD3	4:A:739:EDT:H091	1.42	1.01
1:D:327:LYS:HZ1	4:D:735:EDT:H062	1.26	1.00
1:C:470:ARG:HH11	1:C:470:ARG:HG2	1.23	0.99
1:B:560:PHE:HE2	1:B:563:LYS:HD2	1.25	0.98
1:B:542:MET:CE	1:B:612:LEU:HB3	1.96	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LYS:HG2	3:A:742:CL:CL	2.04	0.94
1:D:324:ARG:HD3	4:D:735:EDT:H022	1.49	0.93
1:D:718:ILE:HG12	1:D:718:ILE:O	1.68	0.91
1:C:372:ILE:HD13	1:C:710:ILE:HG21	1.52	0.89
1:D:327:LYS:NZ	4:D:735:EDT:H062	1.87	0.88
1:A:648:ASP:HB2	1:A:651:LEU:HB3	1.59	0.85
1:D:632:ILE:HG12	1:D:699:CYS:HB3	1.60	0.84
1:D:458:VAL:HG12	1:D:460:MET:HG2	1.58	0.84
1:D:543:TYR:CZ	1:D:545:PRO:HG3	2.13	0.83
1:B:451:LEU:HD12	1:B:451:LEU:H	1.44	0.82
1:B:470:ARG:HH11	1:B:470:ARG:CG	1.93	0.82
1:A:485:PRO:HG3	1:A:509:TYR:CE2	2.16	0.80
1:D:442:THR:HG22	1:D:483:ILE:HD12	1.64	0.80
1:A:456:LYS:HE2	1:A:456:LYS:HA	1.64	0.78
1:A:372:ILE:HD13	1:A:710:ILE:HG21	1.67	0.77
1:B:542:MET:HE1	1:B:612:LEU:CB	2.13	0.75
1:B:470:ARG:HG2	1:B:470:ARG:NH1	1.95	0.75
1:D:426:ARG:HH11	6:D:734:EDO:H21	1.52	0.75
1:A:488:TYR:O	1:A:492:ILE:HG13	1.85	0.75
1:A:451:LEU:H	1:A:451:LEU:HD12	1.52	0.75
1:D:714:ILE:O	1:D:718:ILE:HG22	1.87	0.74
1:C:651:LEU:H	1:C:651:LEU:HD23	1.53	0.73
1:A:338:ARG:HD2	1:A:430:TYR:CD1	2.23	0.73
1:C:316:VAL:HG22	1:D:331:LEU:HD22	1.68	0.73
1:C:722:LEU:O	1:C:723:GLU:HG3	1.89	0.73
1:D:485:PRO:HB2	1:D:486:ASN:ND2	2.04	0.73
1:C:585:TYR:CE2	1:C:586:LEU:HG	2.24	0.72
1:C:383:TYR:CE1	1:C:718:ILE:HD11	2.24	0.72
1:A:353:LYS:HB2	1:A:383:TYR:HD2	1.55	0.71
1:B:372:ILE:HD13	1:B:710:ILE:HG21	1.73	0.71
1:D:325:HIS:CE1	1:D:329:ILE:HD11	2.26	0.70
1:B:703:ASN:ND2	1:B:705:LYS:H	1.90	0.70
1:B:722:LEU:O	1:B:723:GLU:HG3	1.91	0.70
1:B:624:SER:OG	1:B:626:VAL:HG22	1.91	0.69
1:B:511:ARG:HH22	1:B:629:ASP:CG	1.94	0.69
1:B:663:PRO:HG3	1:B:694:PHE:CG	2.28	0.69
1:D:464:THR:OG1	1:D:466:PRO:HD2	1.91	0.69
1:C:665:PRO:HG3	1:C:687:TYR:CE1	2.27	0.69
1:B:703:ASN:HD22	1:B:703:ASN:C	1.96	0.68
1:B:383:TYR:CE2	1:B:718:ILE:HD11	2.29	0.68
1:C:543:TYR:CZ	1:C:545:PRO:HG3	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:THR:HG23	1:A:439:TYR:OH	1.94	0.68
1:C:365:TYR:CE2	1:C:370:LYS:HG3	2.29	0.68
1:C:470:ARG:HH11	1:C:470:ARG:CG	2.02	0.67
1:D:619:LEU:C	1:D:619:LEU:HD23	2.14	0.67
1:B:434:LYS:C	1:B:436:ASN:H	1.98	0.67
1:D:450:ARG:HA	1:D:655:TYR:CE2	2.29	0.67
1:B:543:TYR:CZ	1:B:545:PRO:HG3	2.29	0.67
1:D:372:ILE:HD13	1:D:710:ILE:HG21	1.77	0.66
1:D:564:ILE:HG12	1:D:569:LEU:HD11	1.77	0.66
1:A:569:LEU:HD22	1:A:573:LEU:HD12	1.77	0.66
1:D:436:ASN:HD22	1:D:436:ASN:H	1.43	0.66
1:B:451:LEU:HD12	1:B:451:LEU:N	2.10	0.66
1:C:315:LYS:H	1:C:315:LYS:HD3	1.61	0.66
1:B:485:PRO:HB2	1:B:486:ASN:ND2	2.10	0.65
1:B:619:LEU:HD21	1:B:621:THR:HB	1.78	0.65
1:A:662:LEU:HB2	1:A:663:PRO:HD3	1.78	0.65
1:B:419:SER:HB2	1:B:721:GLN:HE22	1.60	0.65
1:C:613:PHE:HZ	1:C:626:VAL:CG1	2.09	0.65
1:A:722:LEU:O	1:A:723:GLU:HG3	1.96	0.65
1:D:353:LYS:HA	1:D:718:ILE:HD11	1.77	0.65
1:A:314:PHE:HB3	1:C:314:PHE:CZ	2.32	0.65
1:B:540:VAL:HG22	1:B:578:VAL:HG12	1.77	0.65
1:B:561:GLU:HB2	3:B:734:CL:CL	2.34	0.65
1:C:458:VAL:HG12	1:C:460:MET:SD	2.37	0.65
1:C:485:PRO:HG3	1:C:509:TYR:CE2	2.32	0.64
1:B:560:PHE:CE2	1:B:563:LYS:HD2	2.18	0.64
1:C:445:GLY:HA2	1:C:509:TYR:CE2	2.32	0.64
1:B:445:GLY:HA2	1:B:509:TYR:CE2	2.32	0.64
1:A:451:LEU:HD12	1:A:451:LEU:N	2.11	0.64
1:C:675:LYS:O	1:C:678:LYS:HB2	1.98	0.63
1:D:547:TRP:O	1:D:548:ARG:HB3	1.98	0.63
1:D:670:PRO:HD2	1:D:671:TYR:CD2	2.34	0.63
1:A:441:GLN:HG2	1:A:479:TRP:CE2	2.34	0.63
1:D:624:SER:OG	1:D:626:VAL:HG22	1.99	0.62
1:D:669:GLU:HG2	1:D:671:TYR:H	1.63	0.62
1:A:352:PRO:HA	1:A:419:SER:HB3	1.82	0.62
4:A:739:EDT:C1	1:B:324:ARG:HD3	2.30	0.62
1:D:639:PHE:CZ	1:D:663:PRO:HD2	2.35	0.62
1:D:546:THR:OG1	1:D:547:TRP:CD1	2.50	0.61
1:B:703:ASN:HD22	1:B:705:LYS:H	1.49	0.61
4:D:735:EDT:H061	4:D:735:EDT:O20	1.97	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:PHE:O	1:A:476:THR:HG23	2.00	0.61
1:D:365:TYR:CZ	1:D:370:LYS:HG3	2.35	0.61
1:D:447:PRO:HA	5:D:730:C2G:H1G2	1.83	0.61
1:A:320:ARG:HD2	2:A:730:SO4:O4	2.00	0.61
1:C:542:MET:CE	1:C:612:LEU:HB3	2.31	0.61
1:A:561:GLU:HA	3:A:738:CL:CL	2.38	0.60
1:B:582:ARG:NH1	1:B:609:VAL:HG23	2.16	0.60
1:A:324:ARG:HD3	4:A:739:EDT:C9	2.25	0.60
1:C:459:ARG:O	1:C:461:PRO:HD3	2.01	0.60
1:D:482:LEU:HD12	1:D:483:ILE:N	2.16	0.60
1:D:662:LEU:HB2	1:D:663:PRO:HD3	1.83	0.60
1:A:485:PRO:HG3	1:A:509:TYR:CZ	2.36	0.60
1:B:603:VAL:O	1:B:603:VAL:HG13	2.01	0.60
1:D:597:GLU:O	1:D:598:ASN:HB2	2.00	0.60
1:A:597:GLU:O	1:A:598:ASN:HB2	2.01	0.60
1:C:636:PRO:HA	1:C:691:ILE:HD11	1.82	0.60
1:C:639:PHE:CZ	1:C:663:PRO:HD2	2.37	0.59
1:B:450:ARG:HA	1:B:655:TYR:CE2	2.37	0.59
1:D:543:TYR:CE1	1:D:545:PRO:HG3	2.37	0.59
1:C:648:ASP:HB2	1:C:651:LEU:HB3	1.83	0.59
1:C:661:ASP:N	1:C:661:ASP:OD1	2.35	0.59
1:D:532:LEU:O	1:D:533:ASN:HB2	2.03	0.59
4:A:739:EDT:C1	1:B:324:ARG:HH11	2.16	0.59
1:B:548:ARG:HD3	1:B:643:ASP:OD2	2.02	0.59
1:D:705:LYS:O	1:D:708:GLN:HB3	2.02	0.59
1:D:485:PRO:HB2	1:D:486:ASN:HD22	1.67	0.58
1:A:543:TYR:CE2	1:A:545:PRO:HG3	2.38	0.58
1:A:638:PHE:CZ	1:A:683:VAL:HG11	2.38	0.58
1:C:357:PHE:CE1	1:C:373:TYR:HB2	2.38	0.58
1:D:542:MET:HE1	1:D:612:LEU:HD13	1.83	0.58
1:B:365:TYR:CZ	1:B:370:LYS:HG3	2.39	0.58
1:D:639:PHE:CE2	1:D:663:PRO:HD2	2.39	0.58
1:B:714:ILE:O	1:B:718:ILE:HG23	2.03	0.58
1:A:663:PRO:HG3	1:A:694:PHE:CG	2.38	0.58
1:C:383:TYR:CZ	1:C:718:ILE:HD11	2.39	0.58
1:C:662:LEU:HB2	1:C:663:PRO:HD3	1.84	0.58
1:C:434:LYS:C	1:C:436:ASN:H	2.05	0.58
1:C:406:ARG:O	1:C:407:ASN:HB2	2.03	0.57
1:D:325:HIS:CE1	1:D:329:ILE:CD1	2.87	0.57
1:B:638:PHE:HE1	1:B:676:GLU:HG2	1.69	0.57
1:C:662:LEU:CD2	1:C:662:LEU:H	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:TYR:O	1:D:345:ASP:HB2	2.04	0.57
1:A:543:TYR:CZ	1:A:545:PRO:HG3	2.38	0.57
1:B:663:PRO:HG3	1:B:694:PHE:CD1	2.40	0.57
1:D:355:ILE:HD13	1:D:714:ILE:HG21	1.85	0.57
1:D:451:LEU:HD13	1:D:496:ALA:HB1	1.87	0.57
1:C:380:TYR:CE1	1:C:715:HIS:ND1	2.73	0.57
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.03	0.57
1:C:336:LYS:HE2	1:C:337:GLU:OE2	2.05	0.57
1:A:314:PHE:HE2	1:D:330:VAL:O	1.88	0.56
1:A:395:ASN:O	1:A:403:LYS:HE2	2.05	0.56
1:D:444:ASN:C	1:D:511:ARG:HH12	2.07	0.56
1:A:486:ASN:HA	1:A:701:VAL:HG21	1.86	0.56
1:A:703:ASN:H	1:A:703:ASN:HD22	1.53	0.56
1:C:323:LEU:HD23	1:D:327:LYS:HB2	1.87	0.56
1:C:669:GLU:HG2	1:C:671:TYR:H	1.69	0.56
1:D:662:LEU:HB2	1:D:663:PRO:CD	2.35	0.56
1:D:347:GLU:HA	1:D:434:LYS:HD3	1.87	0.56
1:D:451:LEU:HD12	1:D:655:TYR:OH	2.06	0.56
1:D:539:LYS:HB2	1:D:577:TYR:CD1	2.41	0.56
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.70	0.56
1:B:679:ASN:ND2	1:B:682:LYS:HB2	2.20	0.56
1:A:470:ARG:HH11	1:A:470:ARG:CG	2.19	0.56
1:B:488:TYR:OH	1:B:655:TYR:HB2	2.05	0.56
1:D:439:TYR:N	1:D:480:ASP:OD2	2.36	0.55
1:C:420:HIS:CD2	1:C:714:ILE:HG12	2.42	0.55
1:D:338:ARG:HD2	1:D:430:TYR:CD1	2.41	0.55
1:D:465:THR:O	1:D:469:LYS:HG3	2.05	0.55
1:A:434:LYS:C	1:A:436:ASN:H	2.10	0.55
1:A:492:ILE:HD13	1:A:655:TYR:CD2	2.41	0.55
1:A:620:ILE:HD11	1:A:677:LEU:HD21	1.88	0.55
1:D:490:THR:HG23	1:D:504:ILE:HG21	1.88	0.55
1:B:458:VAL:HG13	1:B:460:MET:HE2	1.89	0.55
1:B:353:LYS:HG3	3:B:732:CL:CL	2.44	0.55
1:B:531:HIS:HD2	1:B:531:HIS:O	1.90	0.54
1:C:663:PRO:HG3	1:C:694:PHE:CD2	2.42	0.54
1:A:578:VAL:HG22	1:A:599:PHE:O	2.06	0.54
1:D:356:VAL:HG22	1:D:418:ALA:CB	2.38	0.54
1:D:518:ARG:HD2	1:D:524:TYR:CD2	2.42	0.54
1:C:451:LEU:H	1:C:451:LEU:HD12	1.73	0.54
1:C:316:VAL:HG22	1:D:331:LEU:CD2	2.36	0.54
1:A:355:ILE:HD13	1:A:714:ILE:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:THR:HG22	1:C:483:ILE:HD12	1.88	0.54
1:B:413:GLN:O	1:B:417:GLU:HG3	2.08	0.54
1:B:662:LEU:HB2	1:B:663:PRO:CD	2.38	0.54
1:A:509:TYR:HB3	1:A:511:ARG:HG2	1.89	0.54
1:B:458:VAL:HG12	1:B:458:VAL:O	2.07	0.54
1:C:356:VAL:HG12	1:C:386:ILE:HB	1.90	0.54
1:D:619:LEU:HD23	1:D:620:ILE:N	2.23	0.54
1:B:403:LYS:HE2	3:B:735:CL:CL	2.45	0.53
1:C:364:ASN:HD22	1:C:366:SER:CB	2.20	0.53
1:D:413:GLN:O	1:D:417:GLU:HG3	2.08	0.53
1:D:465:THR:HB	1:D:466:PRO:HD3	1.91	0.53
1:A:542:MET:O	1:A:619:LEU:HD23	2.08	0.53
1:C:365:TYR:CZ	1:C:370:LYS:HG3	2.42	0.53
1:C:418:ALA:O	1:C:437:GLN:HG2	2.09	0.53
1:A:441:GLN:HG2	1:A:479:TRP:CD2	2.43	0.53
1:D:446:THR:O	1:D:625:SER:HB2	2.09	0.53
1:B:356:VAL:HG22	1:B:418:ALA:CB	2.38	0.52
1:A:618:CYS:HB2	1:A:636:PRO:O	2.09	0.52
1:B:538:LYS:HE2	1:B:575:ASP:O	2.10	0.52
1:D:586:LEU:HD23	1:D:586:LEU:O	2.08	0.52
1:C:542:MET:HE2	1:C:612:LEU:HB3	1.90	0.52
1:B:619:LEU:HD23	1:B:619:LEU:C	2.29	0.52
1:C:613:PHE:CZ	1:C:626:VAL:HG12	2.44	0.52
1:C:662:LEU:H	1:C:662:LEU:HD23	1.74	0.52
1:D:354:THR:HG22	1:D:418:ALA:HA	1.91	0.52
1:C:467:LYS:NZ	1:C:470:ARG:HH22	2.07	0.52
1:B:355:ILE:HD13	1:B:714:ILE:HG21	1.92	0.52
1:C:513:ASP:HA	1:C:704:GLY:HA2	1.90	0.52
1:B:485:PRO:HG3	1:B:509:TYR:CE2	2.44	0.52
1:D:438:THR:HA	1:D:480:ASP:OD2	2.10	0.52
1:D:365:TYR:OH	1:D:374:GLU:HG3	2.10	0.52
1:C:639:PHE:CE2	1:C:663:PRO:HD2	2.45	0.51
1:A:325:HIS:NE2	1:A:329:ILE:HD13	2.25	0.51
1:A:357:PHE:CE1	1:A:373:TYR:HB2	2.44	0.51
1:C:648:ASP:O	1:C:649:LYS:HB2	2.11	0.51
1:A:513:ASP:HA	1:A:704:GLY:HA2	1.93	0.51
1:B:383:TYR:CE2	1:B:718:ILE:CD1	2.94	0.51
1:C:484:SER:HB3	1:C:506:GLU:HG2	1.92	0.51
1:C:485:PRO:HD2	1:C:489:SER:HB2	1.92	0.51
1:D:451:LEU:HD12	1:D:451:LEU:H	1.76	0.51
1:C:703:ASN:H	1:C:703:ASN:HD22	1.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:O	1:B:436:ASN:ND2	2.44	0.51
1:C:322:THR:O	1:C:326:VAL:HG23	2.11	0.50
1:D:637:GLN:O	1:D:664:GLY:HA3	2.10	0.50
1:C:613:PHE:HZ	1:C:626:VAL:HG12	1.75	0.50
1:D:542:MET:CE	1:D:612:LEU:HB3	2.40	0.50
1:D:619:LEU:HD21	1:D:621:THR:HB	1.92	0.50
1:C:392:PRO:HB3	1:C:403:LYS:HB3	1.92	0.50
1:D:490:THR:HG23	1:D:504:ILE:HD13	1.92	0.50
1:A:470:ARG:HG2	1:A:470:ARG:NH1	2.25	0.50
1:C:597:GLU:O	1:C:598:ASN:HB2	2.12	0.50
1:A:341:TYR:CD1	1:A:412:TYR:HB3	2.47	0.50
1:C:340:LEU:O	1:C:344:THR:HG23	2.12	0.50
1:C:662:LEU:HB2	1:C:663:PRO:CD	2.41	0.50
1:D:619:LEU:C	1:D:619:LEU:CD2	2.80	0.50
1:B:382:ASN:OD1	1:B:382:ASN:N	2.43	0.49
1:A:639:PHE:CZ	1:A:663:PRO:HD2	2.47	0.49
1:C:350:VAL:HG21	1:C:436:ASN:CG	2.32	0.49
1:C:634:LYS:HE3	1:C:695:TYR:CD1	2.46	0.49
1:A:406:ARG:NH2	3:A:740:CL:CL	2.82	0.49
1:B:363:LYS:HE3	1:B:364:ASN:ND2	2.27	0.49
1:A:331:LEU:CD2	1:B:316:VAL:HG23	2.42	0.49
1:C:526:ASP:O	1:C:530:THR:HG23	2.13	0.49
1:D:324:ARG:HD3	4:D:735:EDT:C2	2.33	0.49
1:D:375:TYR:C	1:D:375:TYR:CD2	2.86	0.49
1:D:383:TYR:CE2	1:D:718:ILE:HD13	2.46	0.49
1:B:343:LEU:HD22	1:D:314:PHE:HE1	1.78	0.49
1:B:531:HIS:O	1:B:531:HIS:CD2	2.65	0.49
1:B:487:ARG:NH1	1:B:506:GLU:OE2	2.45	0.49
1:C:341:TYR:CD1	1:C:412:TYR:HB3	2.48	0.49
1:D:513:ASP:OD2	1:D:707:SER:HB2	2.13	0.49
1:C:372:ILE:CD1	1:C:710:ILE:HG21	2.35	0.49
1:C:448:LEU:HD11	1:C:654:PHE:CD2	2.47	0.49
1:D:404:VAL:O	1:D:404:VAL:HG23	2.12	0.49
1:D:426:ARG:HG2	1:D:475:GLU:HG2	1.95	0.49
1:D:338:ARG:HD2	1:D:430:TYR:CG	2.48	0.49
1:C:377:GLN:HA	1:C:377:GLN:NE2	2.29	0.48
1:A:697:ARG:HD3	1:A:698:PHE:CZ	2.48	0.48
1:B:703:ASN:ND2	1:B:703:ASN:C	2.66	0.48
1:A:420:HIS:HA	1:A:438:THR:O	2.13	0.48
1:C:670:PRO:HD2	1:C:671:TYR:CD2	2.48	0.48
1:D:475:GLU:HA	1:D:475:GLU:OE1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:619:LEU:HD23	1:D:620:ILE:C	2.34	0.48
1:C:663:PRO:HG3	1:C:694:PHE:CG	2.48	0.48
1:D:513:ASP:OD2	1:D:707:SER:CB	2.61	0.48
1:D:673:LEU:HD22	1:D:677:LEU:HD22	1.96	0.48
1:B:647:TYR:O	1:B:648:ASP:HB2	2.14	0.48
1:C:364:ASN:ND2	1:C:366:SER:HB3	2.28	0.48
1:C:620:ILE:HD13	1:C:673:LEU:HD11	1.96	0.48
1:A:548:ARG:HH22	1:A:622:ASP:CG	2.17	0.48
1:A:619:LEU:HB2	1:A:630:TYR:CD2	2.48	0.48
1:D:606:TYR:OH	1:D:611:GLU:OE1	2.27	0.48
1:C:325:HIS:CD2	1:C:329:ILE:HD13	2.49	0.48
1:A:621:THR:O	1:A:639:PHE:HA	2.14	0.48
1:B:325:HIS:CE1	1:B:340:LEU:HB2	2.49	0.48
1:C:467:LYS:HZ1	1:C:470:ARG:HH22	1.59	0.48
1:D:588:SER:O	1:D:591:LEU:HG	2.12	0.48
1:D:697:ARG:HD3	1:D:698:PHE:CZ	2.48	0.48
1:C:582:ARG:NH2	1:C:606:TYR:O	2.46	0.48
1:A:354:THR:HG22	1:A:418:ALA:HB2	1.96	0.48
1:C:347:GLU:HG3	1:C:436:ASN:HB2	1.96	0.48
1:C:363:LYS:HG3	1:C:364:ASN:HB2	1.94	0.48
1:D:673:LEU:O	1:D:677:LEU:HB2	2.14	0.48
1:A:652:ARG:C	1:A:654:PHE:H	2.17	0.47
1:B:472:PHE:CE1	1:B:497:PHE:CE2	3.02	0.47
1:A:602:ASP:OD1	1:A:603:VAL:N	2.47	0.47
1:B:380:TYR:N	1:B:381:PRO:HD3	2.30	0.47
1:D:327:LYS:CE	4:D:735:EDT:H062	2.44	0.47
1:D:439:TYR:CD1	1:D:439:TYR:C	2.87	0.47
1:D:450:ARG:HA	1:D:655:TYR:CZ	2.49	0.47
1:D:572:GLU:OE1	1:D:678:LYS:HE3	2.14	0.47
1:A:324:ARG:CD	4:A:739:EDT:H091	2.29	0.47
1:B:365:TYR:CE2	1:B:370:LYS:HG3	2.49	0.47
1:C:350:VAL:HG21	1:C:436:ASN:OD1	2.15	0.47
1:C:651:LEU:HD23	1:C:651:LEU:N	2.26	0.47
1:C:683:VAL:O	1:C:687:TYR:HB2	2.15	0.47
1:D:470:ARG:CZ	1:D:474:ARG:NH2	2.78	0.47
1:B:519:ALA:HA	1:B:614:LEU:HD22	1.97	0.47
1:B:546:THR:HG23	1:B:624:SER:HB2	1.97	0.47
1:C:353:LYS:HB2	1:C:383:TYR:CD2	2.50	0.47
1:C:559:LEU:HD13	1:C:560:PHE:C	2.35	0.47
1:C:680:LEU:HD23	1:C:680:LEU:HA	1.67	0.47
1:A:324:ARG:HH11	4:A:739:EDT:C10	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:HZ1	4:A:739:EDT:C11	2.28	0.47
1:A:327:LYS:HB2	1:B:323:LEU:HD23	1.97	0.47
1:C:380:TYR:N	1:C:381:PRO:HD3	2.30	0.47
1:C:722:LEU:HD12	1:C:722:LEU:HA	1.75	0.47
4:D:735:EDT:O18	4:D:735:EDT:H042	2.07	0.47
1:B:346:LYS:HE2	1:C:332:ARG:NH2	2.30	0.46
1:B:560:PHE:O	1:B:561:GLU:C	2.53	0.46
1:C:720:GLU:C	1:C:722:LEU:H	2.19	0.46
1:D:452:ALA:H	1:D:455:MET:HE3	1.80	0.46
1:B:405:LYS:O	1:B:411:TYR:HB2	2.15	0.46
1:C:331:LEU:HD22	1:D:316:VAL:HG23	1.97	0.46
1:C:483:ILE:HD11	1:C:710:ILE:HG13	1.97	0.46
1:C:512:ASN:O	1:C:515:LEU:HB2	2.15	0.46
1:A:560:PHE:O	1:A:561:GLU:C	2.53	0.46
1:A:515:LEU:HD12	1:A:632:ILE:HD12	1.97	0.46
4:A:739:EDT:H022	4:A:739:EDT:H072	1.57	0.46
1:C:542:MET:HE1	1:C:612:LEU:HB3	1.95	0.46
1:C:665:PRO:HG3	1:C:687:TYR:CZ	2.50	0.46
1:D:356:VAL:HG13	1:D:386:ILE:HB	1.97	0.46
1:D:546:THR:HG1	1:D:547:TRP:HD1	1.53	0.46
1:D:563:LYS:HG2	1:D:642:TYR:CE2	2.50	0.46
1:B:662:LEU:HB2	1:B:663:PRO:HD3	1.98	0.46
1:C:671:TYR:O	1:C:675:LYS:HG2	2.15	0.46
1:A:450:ARG:HA	1:A:655:TYR:CE2	2.51	0.46
1:C:347:GLU:CG	1:C:436:ASN:HB2	2.46	0.46
1:C:470:ARG:CG	1:C:470:ARG:NH1	2.71	0.46
1:B:488:TYR:O	1:B:492:ILE:HG13	2.16	0.46
1:C:624:SER:OG	1:C:626:VAL:HG23	2.16	0.46
1:A:325:HIS:CE1	1:A:329:ILE:HD13	2.50	0.46
1:A:353:LYS:HB2	1:A:383:TYR:CD2	2.44	0.46
1:A:577:TYR:OH	1:A:680:LEU:HG	2.16	0.46
1:A:639:PHE:CE2	1:A:663:PRO:HD2	2.51	0.46
1:C:559:LEU:CD1	1:C:559:LEU:C	2.85	0.46
1:D:451:LEU:HD12	1:D:451:LEU:N	2.31	0.46
1:A:673:LEU:HD22	1:A:677:LEU:HD22	1.97	0.46
1:C:603:VAL:O	1:C:603:VAL:HG13	2.15	0.46
1:D:472:PHE:O	1:D:476:THR:HG23	2.16	0.46
1:D:576:ASP:HB2	1:D:577:TYR:CD2	2.51	0.46
1:B:387:TRP:HB3	1:B:389:PHE:CE2	2.52	0.45
1:C:364:ASN:HB3	1:C:366:SER:OG	2.16	0.45
1:D:364:ASN:HD22	1:D:366:SER:HB3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ARG:NH2	1:D:474:ARG:HH22	2.13	0.45
1:B:548:ARG:NH2	1:B:622:ASP:OD1	2.39	0.45
1:C:355:ILE:HD13	1:C:714:ILE:HG21	1.98	0.45
1:C:703:ASN:ND2	1:C:705:LYS:H	2.14	0.45
1:A:329:ILE:HG22	1:A:330:VAL:N	2.32	0.45
1:D:488:TYR:OH	1:D:655:TYR:HB2	2.16	0.45
1:D:718:ILE:O	1:D:718:ILE:CG1	2.51	0.45
1:A:368:SER:O	1:A:372:ILE:HG13	2.16	0.45
1:A:483:ILE:HG22	1:A:484:SER:N	2.31	0.45
1:B:451:LEU:N	1:B:451:LEU:CD1	2.77	0.45
1:D:340:LEU:O	1:D:344:THR:HG23	2.17	0.45
1:D:387:TRP:O	1:D:404:VAL:HG22	2.16	0.45
1:D:670:PRO:HD2	1:D:671:TYR:CE2	2.52	0.45
1:B:591:LEU:HD13	1:B:593:LEU:HD21	1.98	0.45
1:D:458:VAL:CG1	1:D:460:MET:HG2	2.39	0.45
1:B:632:ILE:HG12	1:B:699:CYS:HB3	1.99	0.45
1:C:353:LYS:HG2	3:C:731:CL:CL	2.53	0.45
1:C:520:ASN:O	1:C:522:GLN:N	2.50	0.45
1:B:350:VAL:HA	1:B:417:GLU:O	2.17	0.45
1:A:380:TYR:N	1:A:381:PRO:HD3	2.31	0.45
1:C:434:LYS:C	1:C:436:ASN:N	2.70	0.45
1:D:482:LEU:HD12	1:D:483:ILE:H	1.81	0.45
1:B:472:PHE:O	1:B:476:THR:HG23	2.16	0.45
1:C:662:LEU:CD2	1:C:662:LEU:N	2.78	0.45
1:D:663:PRO:HG3	1:D:694:PHE:CG	2.52	0.45
1:A:547:TRP:CG	1:A:548:ARG:N	2.84	0.44
1:B:365:TYR:CE1	1:B:397:VAL:HG13	2.52	0.44
1:D:375:TYR:CE1	1:D:708:GLN:HA	2.51	0.44
1:B:648:ASP:O	1:B:649:LYS:HB2	2.17	0.44
1:A:350:VAL:HA	1:A:417:GLU:O	2.17	0.44
1:A:526:ASP:O	1:A:530:THR:HG23	2.17	0.44
1:B:346:LYS:NZ	1:C:332:ARG:HH22	2.15	0.44
1:C:441:GLN:HG2	1:C:479:TRP:CE2	2.52	0.44
1:C:450:ARG:HA	1:C:655:TYR:CE2	2.53	0.44
1:A:619:LEU:HB2	1:A:630:TYR:CE2	2.51	0.44
1:B:406:ARG:O	1:B:407:ASN:HB2	2.16	0.44
1:B:451:LEU:H	1:B:451:LEU:CD1	2.22	0.44
1:A:658:TYR:O	1:A:662:LEU:HD22	2.18	0.44
1:B:485:PRO:HG3	1:B:509:TYR:CZ	2.52	0.44
1:C:488:TYR:OH	1:C:655:TYR:HB2	2.17	0.44
1:A:646:LYS:O	1:A:648:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:SER:HA	1:B:485:PRO:HD3	1.66	0.44
1:B:569:LEU:HD22	1:B:573:LEU:HD12	2.00	0.44
1:C:325:HIS:NE2	1:C:329:ILE:HD11	2.32	0.44
1:D:443:TRP:HH2	6:D:734:EDO:H12	1.82	0.44
1:D:544:ALA:O	1:D:545:PRO:O	2.35	0.44
1:B:377:GLN:HE21	1:B:377:GLN:CA	2.30	0.44
1:B:461:PRO:C	1:B:463:THR:H	2.21	0.44
1:C:443:TRP:CG	1:C:444:ASN:N	2.86	0.44
1:A:327:LYS:NZ	4:A:739:EDT:N8	2.66	0.44
1:A:382:ASN:OD1	1:A:382:ASN:N	2.51	0.44
1:A:561:GLU:O	1:A:562:LEU:C	2.56	0.44
1:D:338:ARG:HD3	1:D:412:TYR:OH	2.18	0.44
1:D:470:ARG:O	1:D:474:ARG:HG3	2.18	0.44
1:A:662:LEU:HB2	1:A:663:PRO:CD	2.45	0.43
1:B:525:LEU:O	1:B:529:ARG:HG3	2.17	0.43
1:C:338:ARG:HD2	1:C:430:TYR:CD1	2.53	0.43
1:C:644:ILE:C	1:C:646:LYS:H	2.20	0.43
1:D:602:ASP:C	1:D:602:ASP:OD1	2.56	0.43
1:A:435:GLU:O	1:A:435:GLU:HG3	2.17	0.43
1:D:483:ILE:HD11	1:D:710:ILE:HD11	2.00	0.43
1:A:445:GLY:HA2	1:A:509:TYR:CE2	2.54	0.43
1:A:532:LEU:HD21	1:A:606:TYR:CD2	2.53	0.43
1:B:446:THR:HA	1:B:447:PRO:HD3	1.89	0.43
1:D:712:ASP:O	1:D:713:LEU:C	2.55	0.43
1:A:450:ARG:HA	1:A:655:TYR:CZ	2.53	0.43
1:A:487:ARG:HA	1:A:487:ARG:HD3	1.71	0.43
1:B:543:TYR:CE1	1:B:545:PRO:HG3	2.53	0.43
1:C:379:TYR:O	1:C:380:TYR:CG	2.71	0.43
4:D:735:EDT:H021	4:D:735:EDT:H072	1.38	0.43
1:C:370:LYS:HD3	1:C:371:TYR:CE1	2.54	0.43
1:C:459:ARG:O	1:C:459:ARG:HG3	2.18	0.43
1:C:518:ARG:NH2	1:C:524:TYR:CE1	2.86	0.43
1:D:626:VAL:HG12	5:D:730:C2G:HC2	2.00	0.43
1:A:442:THR:HG22	1:A:483:ILE:HD12	2.00	0.43
4:A:739:EDT:O17	1:B:324:ARG:HD3	2.18	0.43
1:B:458:VAL:HG13	1:B:460:MET:CE	2.49	0.43
1:C:499:MET:CE	1:C:503:ARG:HB2	2.49	0.43
1:D:317:ASN:ND2	1:D:320:ARG:HH21	2.16	0.43
1:A:354:THR:HG22	1:A:418:ALA:CB	2.49	0.43
1:A:487:ARG:HH11	1:A:487:ARG:HB2	1.83	0.43
1:D:347:GLU:HG3	1:D:436:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:TYR:HB3	1:B:511:ARG:HG2	1.99	0.43
1:C:446:THR:HA	1:C:447:PRO:HD3	1.92	0.43
1:D:464:THR:HG23	1:D:467:LYS:HB3	2.01	0.43
1:A:406:ARG:O	1:A:407:ASN:HB2	2.19	0.43
1:A:421:TRP:HB2	1:A:439:TYR:HA	2.01	0.43
1:C:566:LEU:HD23	1:C:566:LEU:HA	1.78	0.43
1:C:633:LEU:HB3	1:C:635:ARG:HD3	2.01	0.43
1:D:472:PHE:HB3	1:D:498:TRP:HZ3	1.83	0.43
1:D:521:ASP:OD2	1:D:521:ASP:C	2.57	0.43
1:D:569:LEU:O	1:D:573:LEU:HB2	2.19	0.43
1:A:439:TYR:CD1	1:A:439:TYR:C	2.93	0.42
1:A:551:GLU:OE2	1:A:642:TYR:HE2	2.02	0.42
1:D:624:SER:CB	1:D:626:VAL:HG22	2.49	0.42
1:A:420:HIS:CD2	1:A:714:ILE:HG12	2.54	0.42
1:A:470:ARG:CG	1:A:470:ARG:NH1	2.82	0.42
1:A:703:ASN:HD22	1:A:703:ASN:N	2.17	0.42
1:C:627:MET:HE3	1:C:628:PHE:CZ	2.55	0.42
1:D:470:ARG:NH2	1:D:474:ARG:NH2	2.66	0.42
1:A:451:LEU:N	1:A:451:LEU:CD1	2.80	0.42
1:A:548:ARG:HD3	1:A:643:ASP:OD2	2.19	0.42
1:C:573:LEU:HB3	1:C:577:TYR:HD2	1.83	0.42
1:A:327:LYS:HZ1	4:A:739:EDT:H112	1.85	0.42
1:A:331:LEU:HD21	1:B:316:VAL:HG23	2.02	0.42
1:A:441:GLN:HG2	1:A:479:TRP:CZ2	2.53	0.42
2:A:730:SO4:O1	1:B:327:LYS:HD2	2.18	0.42
1:C:386:ILE:HD12	1:C:414:ALA:HB1	2.02	0.42
1:C:621:THR:OG1	1:C:622:ASP:N	2.51	0.42
1:D:357:PHE:CE1	1:D:373:TYR:HB2	2.54	0.42
1:C:341:TYR:O	1:C:345:ASP:HB2	2.20	0.42
1:D:588:SER:C	1:D:590:ALA:H	2.23	0.42
1:A:335:ASN:O	1:A:338:ARG:N	2.52	0.42
1:A:356:VAL:HG22	1:A:418:ALA:CB	2.49	0.42
1:A:554:SER:C	1:A:556:GLY:H	2.23	0.42
1:B:345:ASP:CG	1:B:434:LYS:HE3	2.39	0.42
1:B:485:PRO:HD2	1:B:489:SER:CB	2.50	0.42
1:D:620:ILE:HD11	1:D:677:LEU:HD21	2.02	0.42
1:D:647:TYR:O	1:D:648:ASP:HB2	2.19	0.42
1:B:639:PHE:CZ	1:B:663:PRO:HD2	2.54	0.42
1:C:359:SER:O	1:C:360:PHE:C	2.56	0.42
1:D:395:ASN:O	1:D:403:LYS:HE2	2.20	0.42
1:C:385:TYR:O	1:C:401:ALA:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PRO:CG	1:A:509:TYR:CE2	2.98	0.41
1:D:485:PRO:HG3	1:D:509:TYR:CE2	2.55	0.41
1:B:561:GLU:O	1:B:562:LEU:C	2.58	0.41
1:C:579:ILE:HG23	1:C:579:ILE:O	2.20	0.41
1:C:582:ARG:NH1	1:C:609:VAL:HB	2.34	0.41
1:C:658:TYR:O	1:C:662:LEU:HD22	2.20	0.41
1:C:675:LYS:O	1:C:678:LYS:N	2.47	0.41
1:D:408:SER:O	1:D:411:TYR:HB3	2.20	0.41
1:D:662:LEU:HD23	1:D:662:LEU:H	1.85	0.41
1:B:354:THR:HG22	1:B:418:ALA:HA	2.02	0.41
1:B:428:PRO:HB3	1:B:430:TYR:CE2	2.55	0.41
1:B:609:VAL:O	1:B:612:LEU:HB2	2.19	0.41
1:D:426:ARG:HD3	6:D:734:EDO:H21	2.02	0.41
1:D:427:THR:HA	1:D:428:PRO:HD3	1.83	0.41
1:B:323:LEU:HD12	1:B:323:LEU:HA	1.74	0.41
1:B:375:TYR:CE1	1:B:708:GLN:HB2	2.56	0.41
1:B:443:TRP:CG	1:B:444:ASN:N	2.88	0.41
1:C:695:TYR:CD2	1:C:695:TYR:C	2.94	0.41
1:A:697:ARG:HD3	1:A:698:PHE:CE2	2.56	0.41
1:C:353:LYS:HB2	1:C:383:TYR:HD2	1.86	0.41
1:C:521:ASP:HB3	1:C:524:TYR:HB3	2.01	0.41
1:C:612:LEU:HD23	1:C:612:LEU:HA	1.78	0.41
1:D:446:THR:HA	1:D:447:PRO:HD3	1.84	0.41
1:B:368:SER:HB3	1:B:510:PRO:HD2	2.02	0.41
1:B:703:ASN:HD22	1:B:704:GLY:N	2.18	0.41
1:C:701:VAL:HG12	1:C:701:VAL:O	2.21	0.41
1:D:662:LEU:HD23	1:D:662:LEU:N	2.35	0.41
1:A:465:THR:HG23	1:A:469:LYS:HE3	2.02	0.41
1:B:572:GLU:HB3	1:B:678:LYS:HE3	2.02	0.41
1:C:483:ILE:HD13	1:C:507:ILE:HD11	2.02	0.41
1:C:588:SER:C	1:C:590:ALA:H	2.22	0.41
1:D:542:MET:HE3	1:D:612:LEU:HB3	2.02	0.41
1:B:367:ASP:O	1:B:370:LYS:HB3	2.21	0.41
1:B:433:LYS:HE2	1:B:433:LYS:O	2.21	0.41
1:C:552:PHE:O	1:C:553:VAL:HG13	2.21	0.41
1:B:338:ARG:HD2	1:B:430:TYR:HB2	2.01	0.41
1:B:376:MET:HE2	1:B:385:TYR:HE1	1.85	0.41
1:B:470:ARG:NH1	1:B:474:ARG:NH1	2.69	0.41
1:B:472:PHE:CE1	1:B:497:PHE:HE2	2.39	0.41
1:C:588:SER:O	1:C:590:ALA:N	2.43	0.41
1:C:624:SER:CB	1:C:626:VAL:HG23	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ILE:O	1:A:591:LEU:HB2	2.21	0.40
1:B:347:GLU:HA	1:B:434:LYS:HD3	2.02	0.40
1:C:684:GLN:O	1:C:688:GLN:HB2	2.21	0.40
1:D:352:PRO:HD2	3:D:732:CL:CL	2.58	0.40
1:D:364:ASN:HB3	1:D:366:SER:HB3	2.04	0.40
1:D:443:TRP:CH2	6:D:734:EDO:H12	2.56	0.40
1:B:420:HIS:HA	1:B:438:THR:O	2.20	0.40
1:C:509:TYR:HA	1:C:510:PRO:HD3	1.95	0.40
1:A:546:THR:HG21	1:A:623:TYR:O	2.22	0.40
1:B:377:GLN:O	1:B:381:PRO:HG3	2.21	0.40
1:D:356:VAL:HG22	1:D:418:ALA:HB2	2.02	0.40
1:D:486:ASN:HA	1:D:701:VAL:HG21	2.02	0.40
1:D:654:PHE:HD2	1:D:658:TYR:HB2	1.85	0.40
1:D:682:LYS:O	1:D:686:GLN:HB2	2.21	0.40
1:A:380:TYR:CE1	1:A:715:HIS:ND1	2.89	0.40
1:A:387:TRP:O	1:A:404:VAL:HG22	2.22	0.40
1:A:406:ARG:HA	1:A:411:TYR:CD1	2.57	0.40
1:C:410:GLU:H	1:C:410:GLU:CD	2.25	0.40
1:C:420:HIS:CE1	1:C:717:ASP:HB3	2.56	0.40
1:D:638:PHE:CE2	1:D:677:LEU:CD1	3.05	0.40
1:A:582:ARG:NH2	1:A:606:TYR:O	2.55	0.40
1:A:641:ALA:HB1	1:A:644:ILE:HB	2.04	0.40
1:A:670:PRO:HD2	1:A:671:TYR:CD2	2.57	0.40
1:A:677:LEU:HD12	1:A:677:LEU:HA	1.98	0.40
1:B:329:ILE:HD12	1:B:336:LYS:HB2	2.04	0.40
1:C:614:LEU:HD23	1:C:614:LEU:HA	1.85	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	408/729 (56%)	372 (91%)	32 (8%)	4 (1%)	15	49
1	B	405/729 (56%)	361 (89%)	34 (8%)	10 (2%)	5	27
1	C	409/729 (56%)	345 (84%)	55 (13%)	9 (2%)	6	29
1	D	389/729 (53%)	342 (88%)	40 (10%)	7 (2%)	8	34
All	All	1611/2916 (55%)	1420 (88%)	161 (10%)	30 (2%)	8	33

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	LEU
1	A	647	TYR
1	B	461	PRO
1	D	547	TRP
1	A	650	GLY
1	C	521	ASP
1	C	561	GLU
1	C	590	ALA
1	B	562	LEU
1	B	565	ASP
1	C	689	GLU
1	D	521	ASP
1	D	533	ASN
1	D	545	PRO
1	A	443	TRP
1	B	345	ASP
1	B	649	LYS
1	B	702	ASP
1	C	506	GLU
1	B	622	ASP
1	C	589	ASN
1	C	647	TYR
1	D	443	TRP
1	D	589	ASN
1	B	443	TRP
1	B	561	GLU
1	C	461	PRO
1	B	535	PRO
1	C	718	ILE
1	D	458	VAL

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	379/675 (56%)	334 (88%)	45 (12%)	5	20
1	B	377/675 (56%)	337 (89%)	40 (11%)	6	26
1	C	379/675 (56%)	333 (88%)	46 (12%)	5	20
1	D	365/675 (54%)	329 (90%)	36 (10%)	8	29
All	All	1500/2700 (56%)	1333 (89%)	167 (11%)	6	24

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	LEU
1	A	339	SER
1	A	348	ASP
1	A	356	VAL
1	A	367	ASP
1	A	382	ASN
1	A	433	LYS
1	A	439	TYR
1	A	451	LEU
1	A	456	LYS
1	A	459	ARG
1	A	460	MET
1	A	470	ARG
1	A	472	PHE
1	A	487	ARG
1	A	488	TYR
1	A	494	ARG
1	A	514	VAL
1	A	537	ASP
1	A	549	ASP
1	A	554	SER
1	A	555	LYS
1	A	559	LEU
1	A	562	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	582	ARG
1	A	591	LEU
1	A	594	SER
1	A	597	GLU
1	A	603	VAL
1	A	607	ASN
1	A	619	LEU
1	A	622	ASP
1	A	623	TYR
1	A	635	ARG
1	A	659	MET
1	A	660	GLU
1	A	662	LEU
1	A	669	GLU
1	A	673	LEU
1	A	678	LYS
1	A	686	GLN
1	A	702	ASP
1	A	703	ASN
1	A	717	ASP
1	A	718	ILE
1	B	323	LEU
1	B	329	ILE
1	B	343	LEU
1	B	356	VAL
1	B	367	ASP
1	B	377	GLN
1	B	382	ASN
1	B	396	VAL
1	B	402	GLU
1	B	450	ARG
1	B	451	LEU
1	B	456	LYS
1	B	457	VAL
1	B	470	ARG
1	B	514	VAL
1	B	533	ASN
1	B	548	ARG
1	B	549	ASP
1	B	559	LEU
1	B	560	PHE
1	B	578	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	585	TYR
1	B	589	ASN
1	B	591	LEU
1	B	594	SER
1	B	597	GLU
1	B	603	VAL
1	B	607	ASN
1	B	609	VAL
1	B	651	LEU
1	B	662	LEU
1	B	669	GLU
1	B	673	LEU
1	B	677	LEU
1	B	702	ASP
1	B	703	ASN
1	B	717	ASP
1	B	718	ILE
1	B	720	GLU
1	B	722	LEU
1	C	315	LYS
1	C	316	VAL
1	C	323	LEU
1	C	332	ARG
1	C	339	SER
1	C	347	GLU
1	C	356	VAL
1	C	359	SER
1	C	382	ASN
1	C	393	ASP
1	C	406	ARG
1	C	450	ARG
1	C	451	LEU
1	C	456	LYS
1	C	457	VAL
1	C	463	THR
1	C	470	ARG
1	C	472	PHE
1	C	482	LEU
1	C	487	ARG
1	C	536	SER
1	C	549	ASP
1	C	559	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	567	ASP
1	C	570	TYR
1	C	576	ASP
1	C	578	VAL
1	C	591	LEU
1	C	597	GLU
1	C	603	VAL
1	C	604	SER
1	C	623	TYR
1	C	626	VAL
1	C	635	ARG
1	C	651	LEU
1	C	656	MET
1	C	660	GLU
1	C	661	ASP
1	C	662	LEU
1	C	669	GLU
1	C	673	LEU
1	C	676	GLU
1	C	678	LYS
1	C	683	VAL
1	C	703	ASN
1	C	722	LEU
1	D	333	ARG
1	D	334	LYS
1	D	336	LYS
1	D	337	GLU
1	D	343	LEU
1	D	356	VAL
1	D	384	ARG
1	D	433	LYS
1	D	436	ASN
1	D	439	TYR
1	D	451	LEU
1	D	456	LYS
1	D	464	THR
1	D	472	PHE
1	D	487	ARG
1	D	500	ASP
1	D	511	ARG
1	D	538	LYS
1	D	546	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	548	ARG
1	D	562	LEU
1	D	576	ASP
1	D	583	MET
1	D	594	SER
1	D	597	GLU
1	D	609	VAL
1	D	622	ASP
1	D	635	ARG
1	D	645	ASP
1	D	647	TYR
1	D	660	GLU
1	D	662	LEU
1	D	673	LEU
1	D	702	ASP
1	D	717	ASP
1	D	718	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	531	HIS
1	A	703	ASN
1	A	708	GLN
1	B	349	ASN
1	B	436	ASN
1	B	517	ASN
1	B	531	HIS
1	B	686	GLN
1	B	703	ASN
1	B	721	GLN
1	C	349	ASN
1	C	364	ASN
1	C	531	HIS
1	C	607	ASN
1	C	686	GLN
1	C	703	ASN
1	D	317	ASN
1	D	413	GLN
1	D	436	ASN
1	D	444	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	686	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 22 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	SO4	A	732	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	C	730	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	B	730	-	4,4,4	0.14	0	6,6,6	0.15	0
4	EDT	A	739	-	7,19,19	0.38	0	12,24,24	1.48	2 (16%)
5	C2G	D	730	-	26,31,31	3.54	9 (34%)	30,46,46	1.41	4 (13%)
6	EDO	D	734	-	3,3,3	0.67	0	2,2,2	0.14	0
2	SO4	D	731	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	A	731	-	4,4,4	0.10	0	6,6,6	0.38	0
4	EDT	D	735	-	7,19,19	0.38	0	12,24,24	1.20	1 (8%)
2	SO4	A	730	-	4,4,4	0.10	0	6,6,6	0.17	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
6	EDO	D	734	-	-	0/1/1/1	-
4	EDT	A	739	-	-	8/13/21/21	-
4	EDT	D	735	-	-	9/13/21/21	-
5	C2G	D	730	-	-	15/22/40/40	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	730	C2G	C6-N1	9.13	1.47	1.35
5	D	730	C2G	C4-N3	8.17	1.48	1.35
5	D	730	C2G	C2-N3	5.85	1.49	1.38
5	D	730	C2G	C6-C5	5.82	1.50	1.38
5	D	730	C2G	O4'-C1'	4.71	1.47	1.41
5	D	730	C2G	PA-O1A	4.32	1.66	1.50
5	D	730	C2G	PB-O1B	4.23	1.65	1.50
5	D	730	C2G	C5-C4	4.06	1.51	1.41
5	D	730	C2G	C4-N4	3.50	1.45	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	730	C2G	C2-N3-C4	4.16	120.56	116.34
5	D	730	C2G	N4-C4-N3	3.42	121.90	116.49
4	A	739	EDT	C1-C2-N3	-3.20	108.93	113.48
4	A	739	EDT	C5-C4-N3	-2.86	109.42	113.48
5	D	730	C2G	C3'-C2'-C1'	2.84	105.26	100.98
4	D	735	EDT	C12-C11-N8	-2.80	109.50	113.48
5	D	730	C2G	PB-O3A-PA	-2.60	123.92	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	739	EDT	C5-C4-N3-C6
4	A	739	EDT	C7-C6-N3-C2
4	D	735	EDT	C5-C4-N3-C6
4	D	735	EDT	C1-C2-N3-C4
4	D	735	EDT	C10-C9-N8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	735	EDT	C12-C11-N8-C9
5	D	730	C2G	C5'-O5'-PA-O1A
5	D	730	C2G	C5'-O5'-PA-O2A
5	D	730	C2G	C5'-O5'-PA-O3A
5	D	730	C2G	PA-O3A-PB-O3B
5	D	730	C2G	C3G-O3B-PB-O1B
5	D	730	C2G	C3G-O3B-PB-O2B
5	D	730	C2G	O1G-C1G-C2G-C3G
4	D	735	EDT	C7-C6-N3-C2
4	A	739	EDT	C12-C11-N8-C9
5	D	730	C2G	O2G-C2G-C3G-O3B
4	A	739	EDT	C6-C7-N8-C9
5	D	730	C2G	C1G-C2G-C3G-O3B
4	A	739	EDT	N3-C6-C7-N8
5	D	730	C2G	O1G-C1G-C2G-O2G
4	D	735	EDT	C1-C2-N3-C6
5	D	730	C2G	O4'-C4'-C5'-O5'
4	D	735	EDT	C10-C9-N8-C11
4	A	739	EDT	C5-C4-N3-C2
5	D	730	C2G	C3'-C4'-C5'-O5'
5	D	730	C2G	PB-O3A-PA-O2A
5	D	730	C2G	C3G-O3B-PB-O3A
4	A	739	EDT	C7-C6-N3-C4
5	D	730	C2G	PB-O3A-PA-O1A
4	D	735	EDT	C7-C6-N3-C4
4	D	735	EDT	C12-C11-N8-C7
4	A	739	EDT	C10-C9-N8-C7

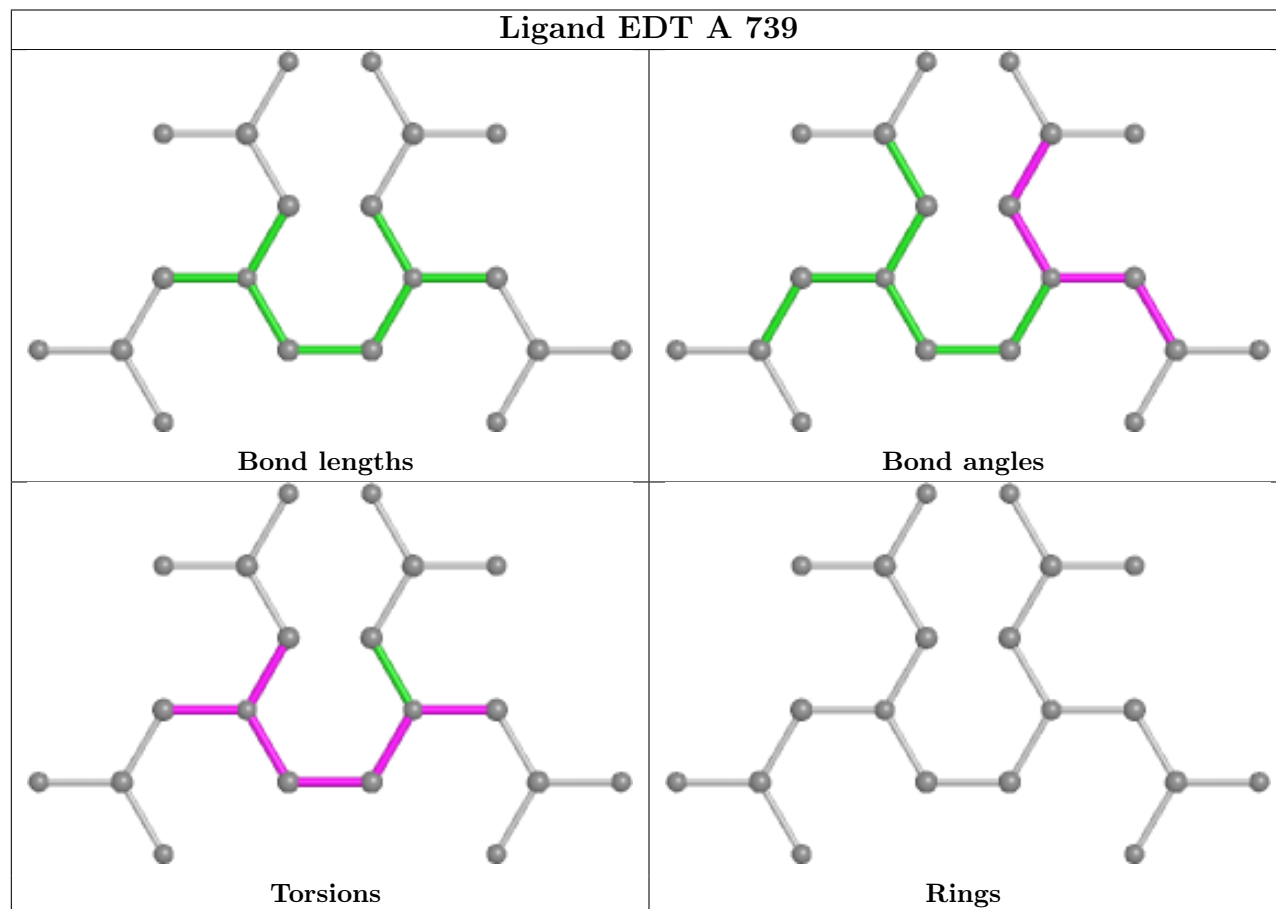
There are no ring outliers.

5 monomers are involved in 27 short contacts:

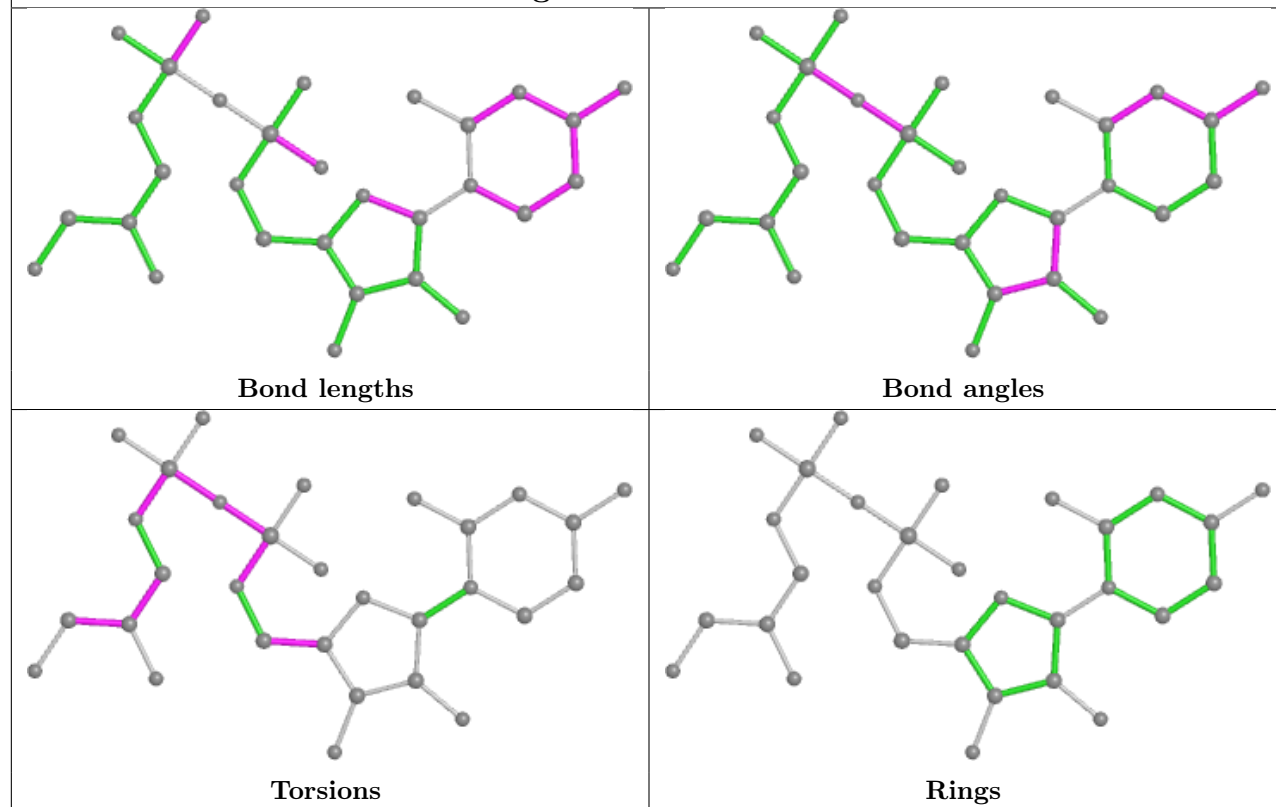
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	739	EDT	11	0
5	D	730	C2G	2	0
6	D	734	EDO	4	0
4	D	735	EDT	8	0
2	A	730	SO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

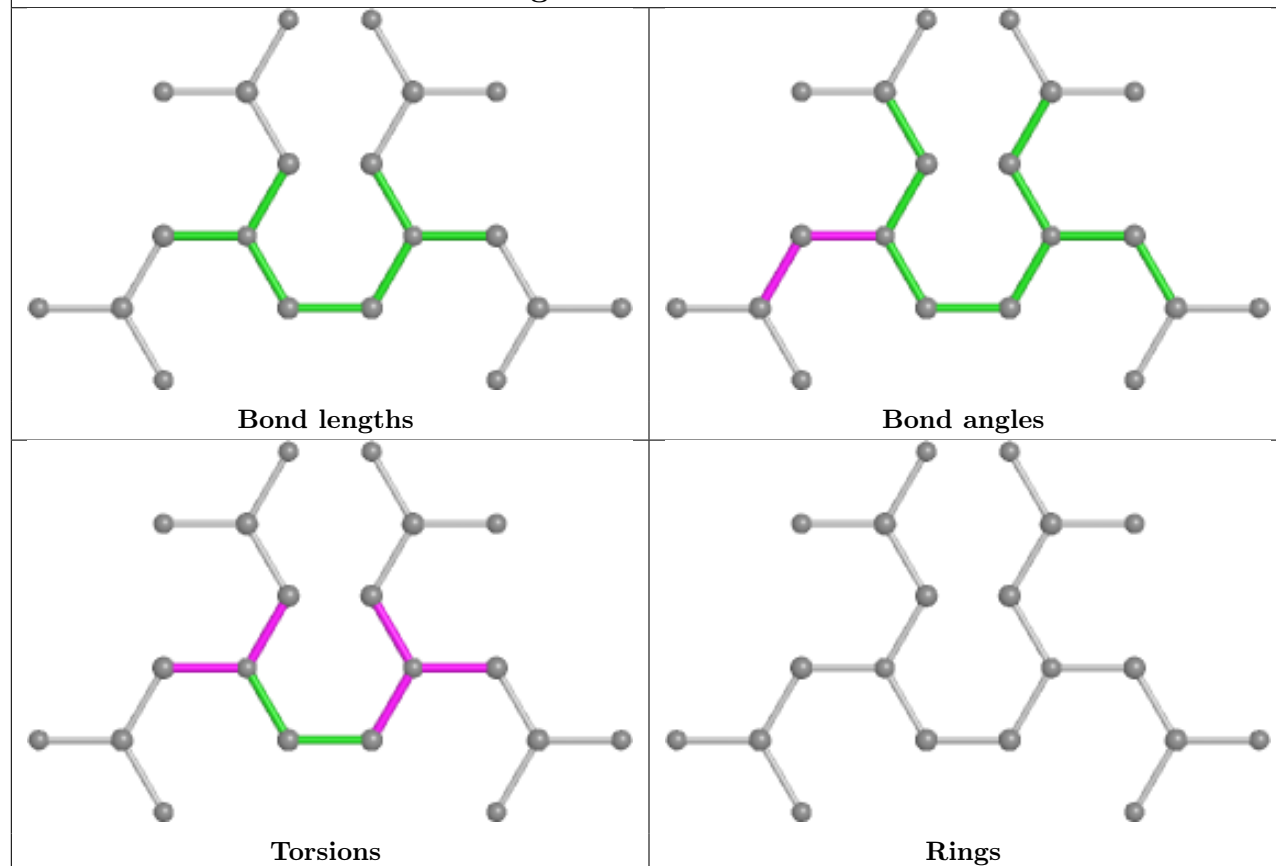
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand C2G D 730



Ligand EDT D 735



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	410/729 (56%)	-0.53	1 (0%) 95 90	63, 83, 152, 220	0
1	B	409/729 (56%)	-0.48	6 (1%) 73 54	68, 87, 148, 219	0
1	C	411/729 (56%)	-0.40	6 (1%) 73 54	71, 93, 175, 251	0
1	D	395/729 (54%)	-0.41	5 (1%) 77 59	68, 92, 147, 253	0
All	All	1625/2916 (55%)	-0.46	18 (1%) 80 64	63, 89, 154, 253	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	585	TYR	4.8
1	A	649	LYS	4.2
1	C	555	LYS	3.9
1	D	724	HIS	3.5
1	C	558	TYR	3.3
1	C	313	ALA	3.0
1	B	652	ARG	3.0
1	D	590	ALA	2.9
1	D	723	GLU	2.8
1	B	554	SER	2.6
1	B	649	LYS	2.6
1	B	537	ASP	2.3
1	C	721	GLN	2.3
1	C	652	ARG	2.1
1	B	555	LYS	2.1
1	B	459	ARG	2.0
1	C	649	LYS	2.0
1	D	584	HIS	2.1

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, 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.

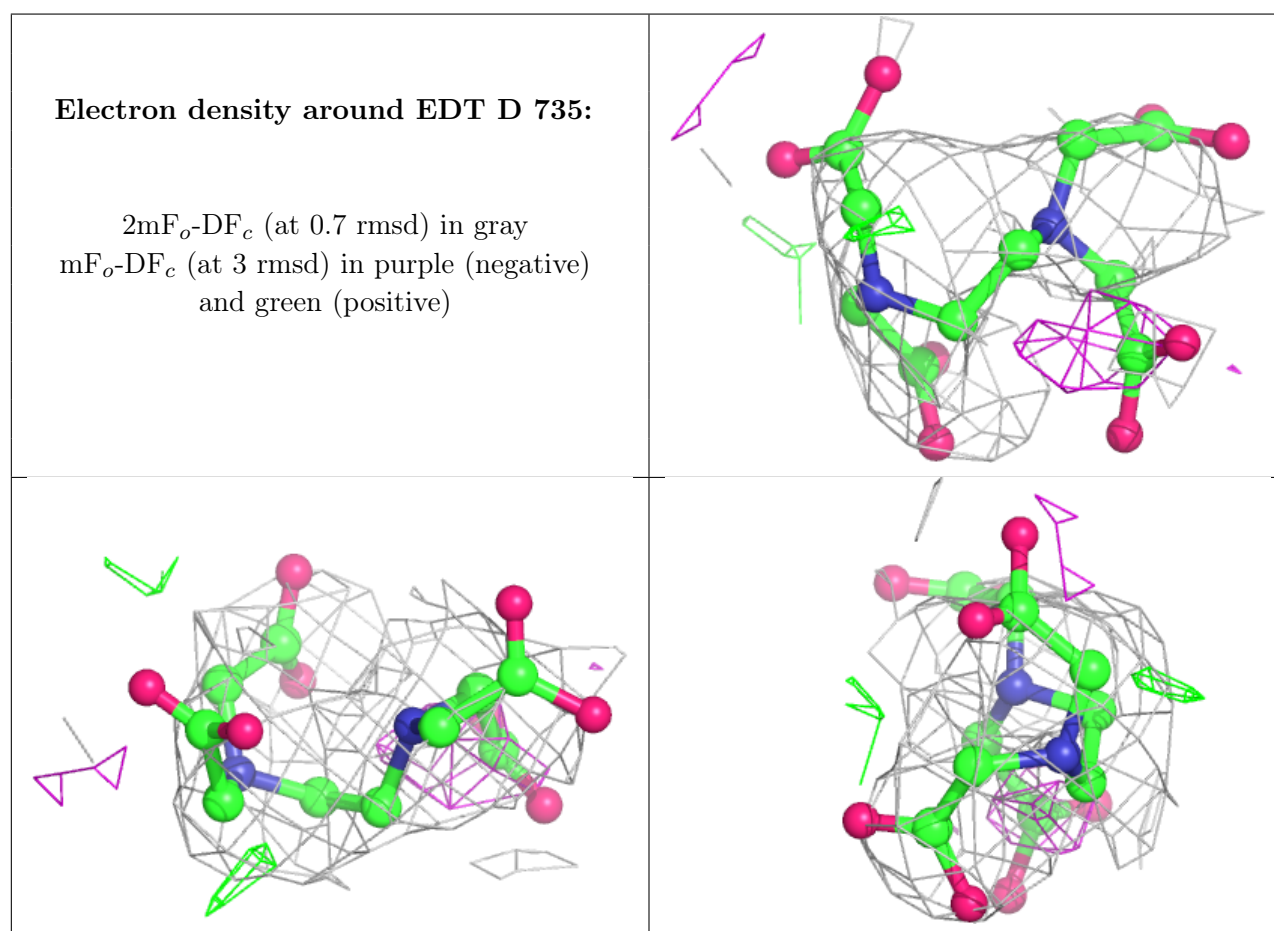
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	D	734	4/4	0.65	0.42	92,92,92,92	0
4	EDT	D	735	20/20	0.69	0.44	170,170,170,170	0
3	CL	B	734	1/1	0.69	0.23	130,130,130,130	0
3	CL	C	734	1/1	0.72	0.41	119,119,119,119	0
4	EDT	A	739	20/20	0.78	0.48	175,175,175,175	0
2	SO4	B	730	5/5	0.82	0.17	177,177,177,177	0
3	CL	A	733	1/1	0.83	0.32	112,112,112,112	0
3	CL	A	737	1/1	0.85	0.14	107,107,107,107	0
3	CL	B	733	1/1	0.85	0.50	121,121,121,121	0
3	CL	C	735	1/1	0.85	0.34	122,122,122,122	0
3	CL	B	735	1/1	0.88	0.72	124,124,124,124	0
2	SO4	A	732	5/5	0.89	0.16	178,178,179,179	0
3	CL	C	731	1/1	0.91	0.13	108,108,108,108	0
3	CL	D	732	1/1	0.91	0.13	93,93,93,93	0
3	CL	D	733	1/1	0.91	0.35	91,91,91,91	0
3	CL	A	736	1/1	0.92	0.19	99,99,99,99	0
3	CL	C	732	1/1	0.93	0.25	114,114,114,114	0
3	CL	A	740	1/1	0.93	0.28	115,115,115,115	0
3	CL	B	732	1/1	0.93	0.33	101,101,101,101	0
3	CL	A	734	1/1	0.93	0.15	106,106,106,106	0
5	C2G	D	730	30/30	0.94	0.18	118,120,121,122	0
3	CL	A	735	1/1	0.95	0.31	103,103,103,103	0
3	CL	C	733	1/1	0.95	0.29	90,90,90,90	0
3	CL	A	741	1/1	0.95	0.08	80,80,80,80	0
3	CL	A	742	1/1	0.95	0.38	99,99,99,99	0
3	CL	A	738	1/1	0.95	0.14	103,103,103,103	0
2	SO4	C	730	5/5	0.96	0.12	120,121,123,123	0

Continued on next page...

Continued from previous page...

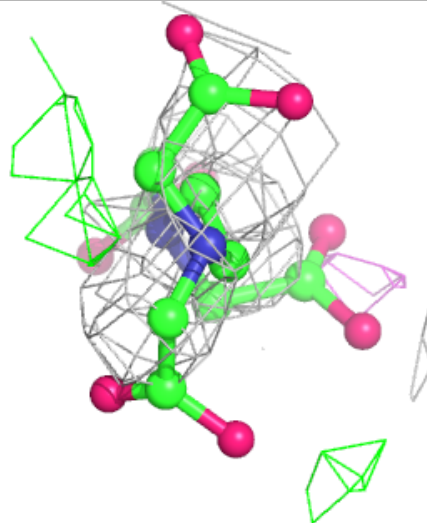
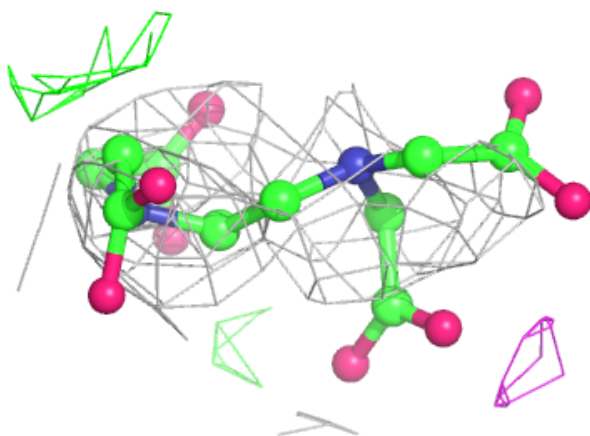
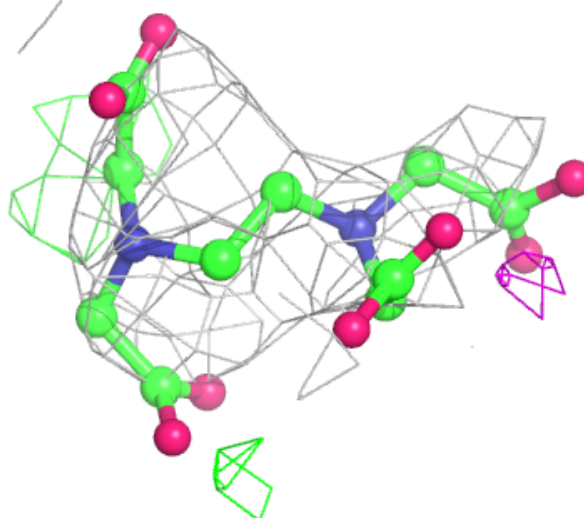
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	B	736	1/1	0.97	0.06	74,74,74,74	0
2	SO4	A	730	5/5	0.97	0.13	115,116,118,120	0
2	SO4	D	731	5/5	0.97	0.10	129,129,131,131	0
2	SO4	A	731	5/5	0.97	0.09	101,101,102,105	0
3	CL	B	731	1/1	0.98	0.13	64,64,64,64	0

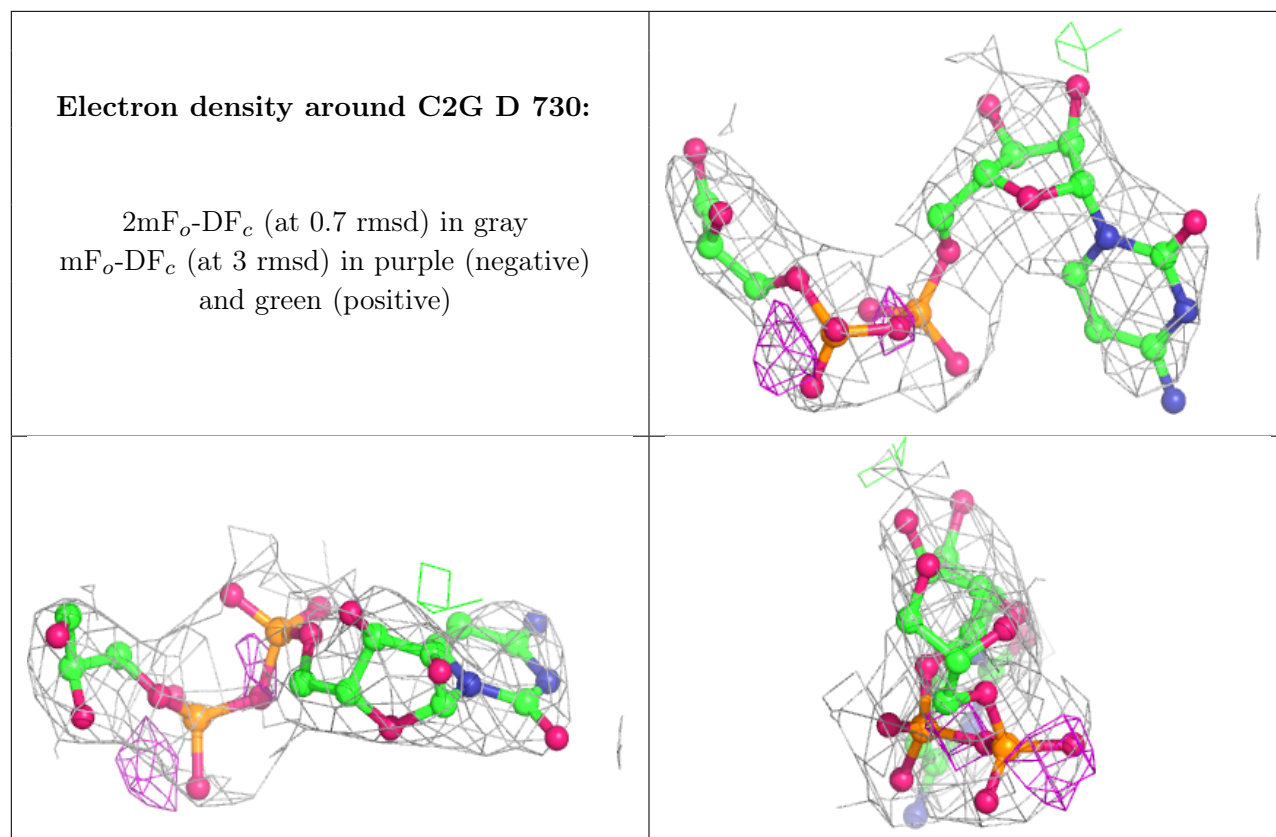
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around EDT A 739:

$2mF_o-DF_c$ (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.