



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:29 AM UTC

PDB ID : 3T6A / pdb_00003t6a
Title : Structure of the C-terminal domain of BCAR3
Authors : Mace, P.D.; Robinson, H.; Riedl, S.J.
Deposited on : 2011-07-28
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

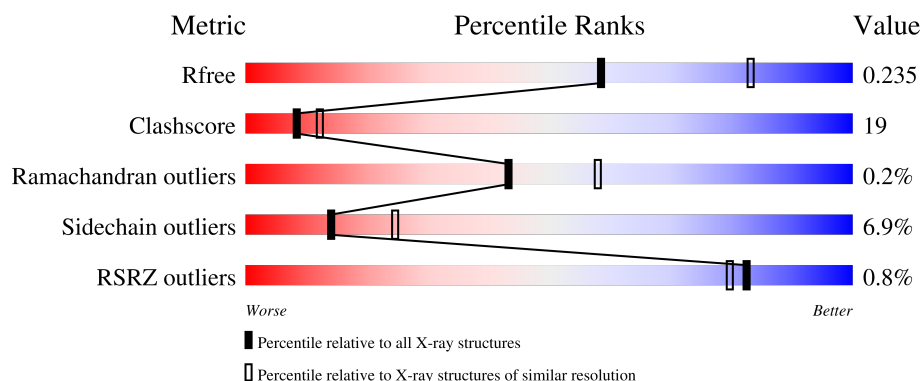
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	333	
1	B	333	
1	C	333	
1	D	333	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10297 atoms, of which 48 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 Breast cancer anti-estrogen resistance protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	H	N	O	S	0	1	0
			2466	1545	12	427	462	20			
1	B	308	Total	C	H	N	O	S	0	3	0
			2480	1557	12	428	463	20			
1	C	308	Total	C	H	N	O	S	0	1	0
			2466	1545	12	427	462	20			
1	D	308	Total	C	H	N	O	S	0	2	0
			2471	1548	12	427	464	20			

There are 40 discrepancies between the modelled and reference sequences:

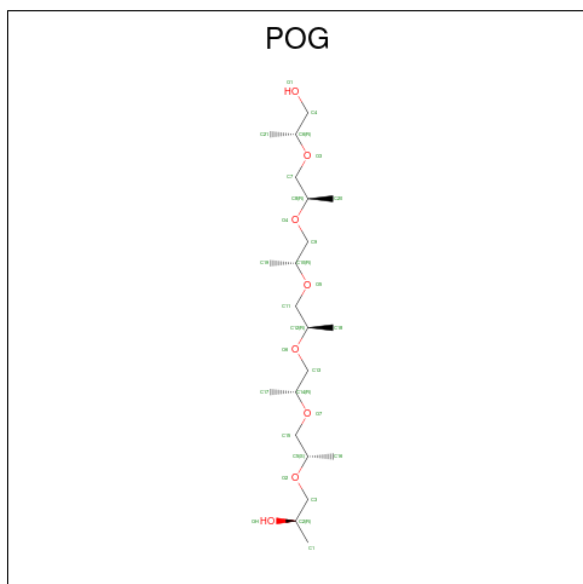
Chain	Residue	Modelled	Actual	Comment	Reference
A	501	MET	-	initiating methionine	UNP O75815
A	536	LEU	MET	engineered mutation	UNP O75815
A	826	LEU	-	expression tag	UNP O75815
A	827	GLU	-	expression tag	UNP O75815
A	828	HIS	-	expression tag	UNP O75815
A	829	HIS	-	expression tag	UNP O75815
A	830	HIS	-	expression tag	UNP O75815
A	831	HIS	-	expression tag	UNP O75815
A	832	HIS	-	expression tag	UNP O75815
A	833	HIS	-	expression tag	UNP O75815
B	501	MET	-	initiating methionine	UNP O75815
B	536	LEU	MET	engineered mutation	UNP O75815
B	826	LEU	-	expression tag	UNP O75815
B	827	GLU	-	expression tag	UNP O75815
B	828	HIS	-	expression tag	UNP O75815
B	829	HIS	-	expression tag	UNP O75815
B	830	HIS	-	expression tag	UNP O75815
B	831	HIS	-	expression tag	UNP O75815
B	832	HIS	-	expression tag	UNP O75815
B	833	HIS	-	expression tag	UNP O75815
C	501	MET	-	initiating methionine	UNP O75815

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Chain	Residue	Modelled	Actual	Comment	Reference
C	536	LEU	MET	engineered mutation	UNP O75815
C	826	LEU	-	expression tag	UNP O75815
C	827	GLU	-	expression tag	UNP O75815
C	828	HIS	-	expression tag	UNP O75815
C	829	HIS	-	expression tag	UNP O75815
C	830	HIS	-	expression tag	UNP O75815
C	831	HIS	-	expression tag	UNP O75815
C	832	HIS	-	expression tag	UNP O75815
C	833	HIS	-	expression tag	UNP O75815
D	501	MET	-	initiating methionine	UNP O75815
D	536	LEU	MET	engineered mutation	UNP O75815
D	826	LEU	-	expression tag	UNP O75815
D	827	GLU	-	expression tag	UNP O75815
D	828	HIS	-	expression tag	UNP O75815
D	829	HIS	-	expression tag	UNP O75815
D	830	HIS	-	expression tag	UNP O75815
D	831	HIS	-	expression tag	UNP O75815
D	832	HIS	-	expression tag	UNP O75815
D	833	HIS	-	expression tag	UNP O75815

- Molecule 2 is (20S)-2,5,8,11,14,17-HEXAMETHYL-3,6,9,12,15,18-HEXAAXAHENICOSAN E-1,20-DIOL (CCD ID: POG) (formula: C₂₁H₄₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	12	4		

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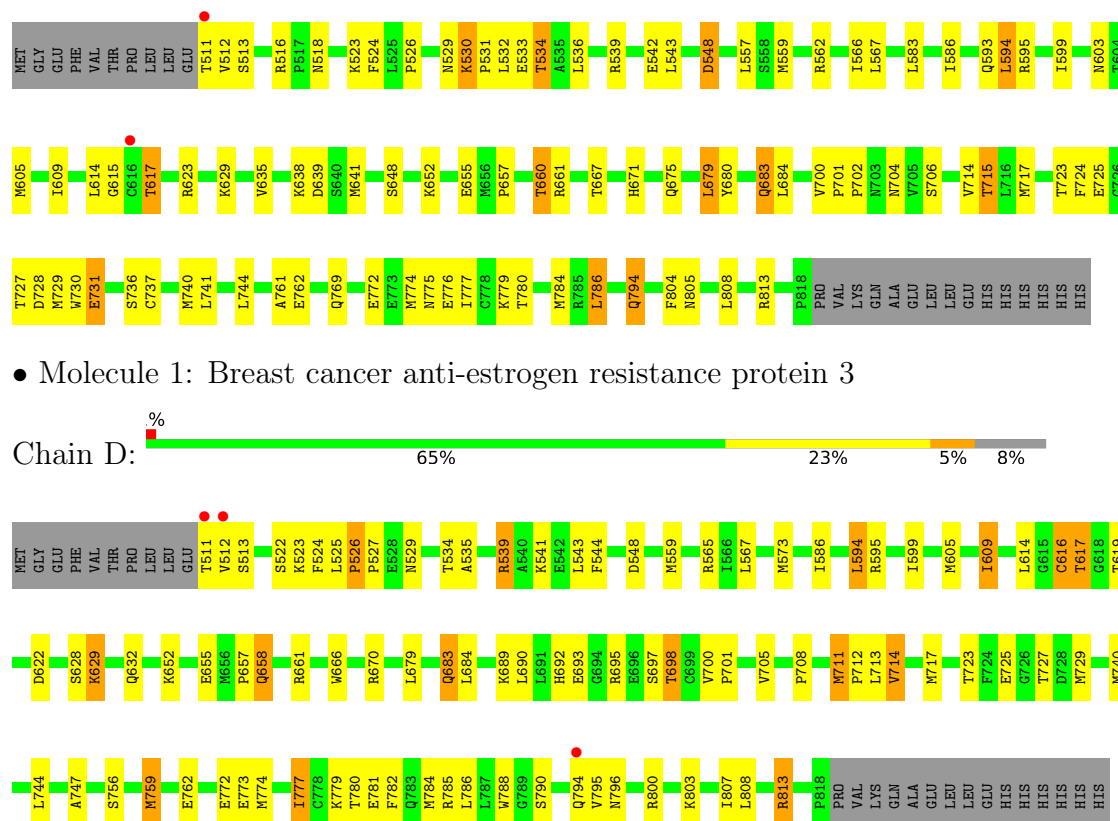
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			17	12	5		

- Molecule 3 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	8	Total	X	0	0
			8	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	105	Total	O	0	0
			105	105		
4	C	87	Total	O	0	0
			87	87		
4	D	88	Total	O	0	0
			88	88		



• Molecule 1: Breast cancer anti-estrogen resistance protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.23Å 151.89Å 196.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.40 19.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (19.76-2.40) 98.4 (19.76-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.174 , 0.244 0.169 , 0.235	Depositor DCC
R_{free} test set	2942 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.7	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	0.96	EDS
Total number of atoms	10297	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2527e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UNX, POG

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	0.51	0/2500	0.83	4/3376 (0.1%)
1	B	0.51	0/2521	0.79	0/3404
1	C	0.52	0/2500	0.80	2/3376 (0.1%)
1	D	0.50	0/2508	0.82	3/3387 (0.1%)
All	All	0.51	0/10029	0.81	9/13543 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ARG	CA-C-N	6.73	126.52	119.05
1	A	516	ARG	C-N-CA	6.73	126.52	119.05
1	D	526	PRO	CA-C-N	6.25	125.74	119.24
1	D	526	PRO	C-N-CA	6.25	125.74	119.24
1	D	705	VAL	N-CA-C	5.56	115.90	108.11
1	C	516	ARG	CA-C-N	5.51	125.34	119.28
1	C	516	ARG	C-N-CA	5.51	125.34	119.28
1	A	659	ILE	N-CA-C	-5.35	107.21	111.81
1	A	674	THR	N-CA-C	5.30	117.47	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2454	12	2484	103	0
1	B	2468	12	2501	115	0
1	C	2454	12	2484	87	0
1	D	2459	12	2488	93	0
2	A	16	0	23	0	0
2	B	17	0	24	7	0
3	D	8	0	0	0	0
4	A	93	0	0	7	0
4	B	105	0	0	12	0
4	C	87	0	0	5	0
4	D	88	0	0	8	0
All	All	10249	48	10004	379	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 (379) 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:D:619:THR:HG23	1:D:622[B]:ASP:H	1.04	1.16
1:D:619:THR:HG23	1:D:622[A]:ASP:H	1.05	1.16
1:C:744:LEU:HD12	1:D:744:LEU:HD12	1.19	1.15
1:A:744:LEU:HD12	1:B:744:LEU:HD12	1.29	1.15
1:D:813:ARG:HH11	1:D:813:ARG:HG2	1.11	1.15
1:D:539:ARG:HH11	1:D:539:ARG:HG2	1.06	1.13
1:B:702:PRO:HA	1:D:759:MET:HG3	1.30	1.13
1:C:729:MET:HE2	1:C:729:MET:HA	1.33	1.10
1:C:559:MET:HE3	4:C:920:HOH:O	1.60	1.01
1:C:530:LYS:HB2	1:C:531:PRO:HD2	1.42	1.01
1:C:744:LEU:CD1	1:D:744:LEU:HD12	1.92	0.99
1:A:543:LEU:HD11	1:A:773:GLU:HG2	1.45	0.97
1:D:573:MET:HE3	4:D:910:HOH:O	1.65	0.97
1:D:679:LEU:HD12	1:D:683:GLN:HG3	1.46	0.96
1:B:715:THR:HG23	1:B:730:TRP:HE1	1.32	0.94
1:A:748:ARG:HB2	4:B:845:HOH:O	1.67	0.94
1:B:748:ARG:HH11	1:B:748:ARG:HG2	1.30	0.93
1:C:559:MET:HE2	1:C:779:LYS:HA	1.51	0.92
1:C:744:LEU:HD12	1:D:744:LEU:CD1	2.00	0.90
1:B:529:ASN:ND2	1:B:785:ARG:HH21	1.70	0.90
1:B:702:PRO:HA	1:D:759:MET:CG	2.02	0.89
1:D:539:ARG:HG2	1:D:539:ARG:NH1	1.82	0.88
1:B:540:ALA:HB1	1:B:777:ILE:HD11	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:813:ARG:HG2	1:D:813:ARG:NH1	1.86	0.87
1:B:529:ASN:HD22	1:B:785:ARG:HH21	1.20	0.86
1:D:511:THR:HG22	1:D:512:VAL:H	1.39	0.86
1:B:512:VAL:HG22	1:B:513:SER:H	1.41	0.85
1:D:658:GLN:HE21	1:D:658:GLN:H	1.22	0.85
1:C:559:MET:HE1	1:C:779:LYS:HG2	1.58	0.85
1:A:717:MET:HE3	1:B:740:MET:HE1	1.59	0.84
1:A:512:VAL:HG22	1:A:513:SER:H	1.42	0.84
1:A:541:LYS:HD3	1:A:616:CYS:CB	2.09	0.83
1:A:559:MET:HE2	1:A:779:LYS:HA	1.59	0.83
1:C:683:GLN:HE21	1:C:683:GLN:HA	1.44	0.83
1:B:748:ARG:HH11	1:B:748:ARG:CG	1.92	0.82
1:A:541:LYS:HD3	1:A:616:CYS:HB3	1.61	0.81
1:A:809:THR:O	1:A:813:ARG:HG3	1.80	0.81
1:C:559:MET:CE	1:C:779:LYS:HG2	2.11	0.81
1:A:729:MET:HA	1:A:729:MET:HE2	1.61	0.81
1:C:562:ARG:HH22	1:C:775:ASN:HD21	1.25	0.81
1:B:562:ARG:HH12	1:B:775:ASN:HD21	1.29	0.80
1:C:635:VAL:CG2	1:C:679:LEU:HD21	2.11	0.80
1:D:658:GLN:H	1:D:658:GLN:NE2	1.80	0.80
1:C:661:ARG:NH2	1:C:813:ARG:HA	1.98	0.78
1:A:511:THR:HG22	1:A:512:VAL:H	1.48	0.78
1:B:715:THR:CG2	1:B:730:TRP:HE1	1.96	0.78
1:B:658:GLN:H	1:B:658:GLN:HE21	1.30	0.78
1:A:529:ASN:HD21	1:A:785:ARG:HE	1.30	0.78
1:B:657:PRO:HA	1:B:660:THR:HG22	1.66	0.77
1:B:679:LEU:HD12	1:B:683:GLN:HG3	1.66	0.77
1:D:544:PHE:O	1:D:629:LYS:HE3	1.84	0.77
1:D:617:THR:HG22	1:D:622[B]:ASP:OD2	1.84	0.76
1:A:658:GLN:H	1:A:658:GLN:HE21	1.30	0.76
1:B:748:ARG:HG2	1:B:748:ARG:NH1	1.92	0.76
1:B:574:ARG:HD3	1:B:580:SER:HA	1.68	0.76
1:B:670:ARG:HH21	1:B:678:ILE:HG12	1.51	0.75
1:A:530:LYS:HG2	1:A:533:GLU:HG3	1.68	0.75
1:A:744:LEU:HD12	1:B:744:LEU:CD1	2.12	0.75
1:C:744:LEU:HD21	1:D:740:MET:HE2	1.69	0.74
1:B:737:CYS:HA	1:B:740:MET:HE3	1.70	0.74
1:C:729:MET:HA	1:C:729:MET:CE	2.15	0.73
1:D:729:MET:HE2	1:D:729:MET:HA	1.69	0.73
1:C:737:CYS:HA	1:C:740:MET:HE3	1.70	0.73
1:D:666:TRP:HB3	1:D:670:ARG:HH12	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASN:ND2	1:A:785:ARG:HE	1.86	0.73
1:A:759:MET:HG3	1:C:702:PRO:HA	1.70	0.72
1:B:658:GLN:H	1:B:658:GLN:NE2	1.86	0.72
1:A:715:THR:HG22	1:A:730:TRP:HE1	1.54	0.72
1:B:619:THR:HG22	1:B:622:ASP:OD2	1.90	0.72
1:D:619:THR:HG22	1:D:622[A]:ASP:OD1	1.90	0.72
1:C:559:MET:CE	1:C:779:LYS:HA	2.21	0.71
1:B:512:VAL:HG22	1:B:513:SER:N	2.05	0.70
1:C:533:GLU:HB2	1:C:536:LEU:HD12	1.71	0.70
1:B:652:LYS:HE3	1:B:727:THR:OG1	1.91	0.70
1:A:740:MET:HE1	1:B:717:MET:HG2	1.74	0.70
1:C:512:VAL:HG22	1:C:513:SER:H	1.56	0.70
1:C:530:LYS:HB2	1:C:531:PRO:CD	2.19	0.70
1:D:701:PRO:HB2	4:D:844:HOH:O	1.91	0.70
1:D:683:GLN:HE21	1:D:683:GLN:HA	1.56	0.69
1:C:567:LEU:HD21	1:C:762:GLU:HG3	1.73	0.68
1:C:774:MET:O	1:C:777:ILE:HG22	1.92	0.68
1:A:737:CYS:HA	1:A:740:MET:CE	2.23	0.67
1:C:715:THR:HG21	1:C:728:ASP:HB3	1.77	0.67
1:D:619:THR:HG22	1:D:622[A]:ASP:CG	2.19	0.67
1:A:744:LEU:CD1	1:B:740:MET:HB3	2.24	0.67
1:A:530:LYS:CG	1:A:533:GLU:HG3	2.25	0.67
1:D:655:GLU:HG3	4:D:848:HOH:O	1.94	0.66
1:C:635:VAL:HG21	1:C:679:LEU:HD21	1.76	0.66
1:B:559:MET:HE2	4:B:837:HOH:O	1.94	0.66
1:D:813:ARG:HH11	1:D:813:ARG:CG	1.98	0.66
1:A:715:THR:HG21	1:A:728:ASP:O	1.96	0.65
1:A:759:MET:CG	1:C:702:PRO:HA	2.27	0.65
1:D:679:LEU:CD1	1:D:683:GLN:HG3	2.23	0.65
1:A:541:LYS:HD3	1:A:616:CYS:HB2	1.79	0.65
1:B:590:HIS:H	1:B:590:HIS:CD2	2.14	0.65
1:C:559:MET:HE2	1:C:779:LYS:CA	2.24	0.64
1:D:619:THR:CG2	1:D:622[A]:ASP:CG	2.70	0.64
1:B:712:PRO:O	1:B:715:THR:HG22	1.96	0.64
1:D:666:TRP:HB3	1:D:670:ARG:NH1	2.12	0.64
1:B:653:ALA:HA	1:B:656:MET:HE3	1.79	0.64
1:B:711:MET:HB3	1:B:712:PRO:HD3	1.77	0.64
1:B:512:VAL:O	1:B:593:GLN:NE2	2.30	0.64
1:D:559:MET:HE2	1:D:779:LYS:HG2	1.78	0.64
1:A:590:HIS:CD2	1:A:590:HIS:H	2.14	0.64
1:A:593:GLN:HA	1:A:593:GLN:HE21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:LYS:HE3	1:C:727:THR:OG1	1.98	0.63
1:C:740:MET:HE1	1:D:717:MET:HE3	1.79	0.63
1:B:715:THR:HG23	1:B:730:TRP:NE1	2.09	0.63
1:A:512:VAL:HG22	1:A:513:SER:N	2.14	0.63
1:A:559:MET:HE1	4:A:843:HOH:O	1.98	0.62
1:B:512:VAL:HG13	1:B:513:SER:O	1.99	0.62
1:B:675[B]:GLN:CD	1:B:675[B]:GLN:H	2.07	0.62
1:C:683:GLN:HE21	1:C:683:GLN:CA	2.13	0.62
1:D:524:PHE:HE2	1:D:772:GLU:HG2	1.64	0.62
1:C:724:PHE:CE1	1:C:725:GLU:HG3	2.34	0.61
1:B:539:ARG:HD2	1:B:539:ARG:O	2.00	0.61
1:A:525:LEU:HD13	1:A:782:PHE:CE1	2.35	0.61
1:A:737:CYS:HA	1:A:740:MET:HE2	1.82	0.61
1:D:692:HIS:HD2	4:D:908:HOH:O	1.83	0.61
1:C:511:THR:HG21	1:C:593:GLN:HE22	1.64	0.61
1:A:529:ASN:HD22	1:A:785:ARG:HH21	1.49	0.61
1:B:614:LEU:HD21	1:B:662:LEU:HD11	1.82	0.61
1:B:655:GLU:HG3	4:B:843:HOH:O	2.00	0.60
1:D:559:MET:CE	1:D:779:LYS:HG2	2.31	0.60
1:B:670:ARG:HH21	1:B:678:ILE:CG1	2.12	0.60
1:D:544:PHE:CZ	1:D:777:ILE:HD13	2.37	0.59
1:C:529:ASN:HA	1:C:533:GLU:OE2	2.02	0.59
1:C:534:THR:HG23	4:C:900:HOH:O	2.01	0.59
1:A:530:LYS:HG2	1:A:533:GLU:CG	2.32	0.59
1:A:524:PHE:HE2	1:A:772:GLU:HG2	1.66	0.59
1:A:704:ASN:ND2	1:C:704:ASN:HD22	2.01	0.59
1:A:736:SER:HB3	1:A:739:ILE:HD13	1.84	0.59
1:A:599:ILE:HA	1:A:711:MET:HE1	1.84	0.59
1:A:715:THR:HG22	1:A:730:TRP:NE1	2.17	0.59
1:D:511:THR:HG22	1:D:512:VAL:N	2.16	0.58
1:A:744:LEU:HD11	1:B:740:MET:HB3	1.84	0.58
1:B:524:PHE:CD1	1:B:773:GLU:HG3	2.39	0.58
1:C:635:VAL:HG22	1:C:679:LEU:HD21	1.85	0.57
1:D:512:VAL:HG22	1:D:513:SER:H	1.70	0.57
1:C:599:ILE:HD11	1:C:714:VAL:HG12	1.87	0.57
1:B:745:ALA:CB	2:B:834:POG:H162	2.35	0.57
1:D:614:LEU:HD12	1:D:808:LEU:HD22	1.85	0.56
1:A:579:VAL:HG11	1:A:584:GLU:HG2	1.88	0.56
1:B:619:THR:HG22	1:B:622:ASP:CG	2.31	0.56
1:C:675:GLN:HA	1:C:675:GLN:NE2	2.20	0.56
1:D:567:LEU:HD21	1:D:762:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASN:HD21	1:A:794:GLN:HB2	1.71	0.56
1:D:785:ARG:HD2	1:D:790:SER:HA	1.88	0.55
1:B:540:ALA:CB	1:B:777:ILE:HD11	2.32	0.55
1:C:657:PRO:HA	1:C:660:THR:HG22	1.88	0.55
1:B:528:GLU:HG3	1:B:790:SER:OG	2.07	0.55
1:D:539:ARG:NH1	1:D:539:ARG:CG	2.60	0.55
1:A:518:ASN:ND2	1:A:794:GLN:HB2	2.22	0.55
1:A:713:LEU:HD13	1:A:747:ALA:HB2	1.87	0.55
1:C:559:MET:HE2	1:C:779:LYS:CG	2.36	0.55
1:D:512:VAL:HG22	1:D:513:SER:N	2.22	0.54
1:A:675:GLN:NE2	4:A:927:HOH:O	2.36	0.54
1:C:511:THR:HG21	1:C:593:GLN:NE2	2.22	0.54
1:D:813:ARG:NH1	1:D:813:ARG:CG	2.61	0.54
1:A:555:HIS:CG	1:A:774:MET:HG2	2.42	0.54
1:C:638:LYS:HG2	1:C:639:ASP:OD1	2.08	0.54
1:D:565:ARG:HD3	1:D:573:MET:SD	2.48	0.54
1:A:655:GLU:HG3	4:A:846:HOH:O	2.08	0.53
1:A:736:SER:CB	1:A:739:ILE:HD13	2.38	0.53
1:C:518:ASN:HB2	1:C:794:GLN:HE22	1.72	0.53
1:C:667:THR:HG23	1:C:671:HIS:CE1	2.44	0.53
1:B:702:PRO:HD3	1:D:759:MET:HE3	1.90	0.53
1:A:722:VAL:HA	4:A:874:HOH:O	2.07	0.53
1:C:635:VAL:HG21	1:C:679:LEU:CD2	2.37	0.53
1:D:559:MET:HE2	1:D:779:LYS:CG	2.39	0.53
1:D:679:LEU:HD12	1:D:683:GLN:CG	2.31	0.53
1:A:541:LYS:HD2	1:A:612:ASP:OD1	2.09	0.53
1:A:574:ARG:HB2	1:A:574:ARG:CZ	2.39	0.53
1:A:739:ILE:HD12	1:A:739:ILE:H	1.74	0.53
1:A:744:LEU:HD13	1:B:740:MET:HB3	1.88	0.53
1:D:658:GLN:HE21	1:D:658:GLN:N	2.00	0.53
1:A:512:VAL:HG13	1:A:513:SER:O	2.09	0.53
1:C:559:MET:CE	1:C:779:LYS:CG	2.86	0.53
1:D:599:ILE:HG13	1:D:714:VAL:HG11	1.90	0.53
1:B:780:THR:O	1:B:784:MET:HG3	2.09	0.53
1:D:652:LYS:HE3	1:D:727:THR:OG1	2.09	0.53
1:C:740:MET:HE1	1:D:717:MET:HG2	1.90	0.52
1:B:511:THR:CG2	4:B:894:HOH:O	2.57	0.52
1:A:512:VAL:O	1:A:593:GLN:NE2	2.42	0.52
1:A:574:ARG:HB2	1:A:574:ARG:NH1	2.23	0.52
1:D:782:PHE:HE2	1:D:786:LEU:HD11	1.74	0.52
1:C:532:LEU:HD21	1:C:804:PHE:HZ	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:MET:O	1:D:609:ILE:HG12	2.09	0.52
1:B:619:THR:HG23	1:B:622:ASP:H	1.74	0.52
1:C:661:ARG:HH21	1:C:813:ARG:HA	1.73	0.52
1:B:635:VAL:HG21	1:B:679:LEU:HD21	1.92	0.52
1:B:745:ALA:HB1	2:B:834:POG:H162	1.91	0.52
1:A:795:VAL:HG12	1:A:796:ASN:N	2.23	0.52
1:B:540:ALA:HB1	1:B:777:ILE:CD1	2.32	0.51
1:C:715:THR:CG2	1:C:730:TRP:HE1	2.24	0.51
1:B:595:ARG:HG2	1:B:714:VAL:HG22	1.92	0.51
1:B:661:ARG:NH2	1:B:813:ARG:HA	2.26	0.51
1:A:614:LEU:HD23	1:A:815:LEU:HD12	1.92	0.51
1:B:655:GLU:HG2	4:B:869:HOH:O	2.09	0.51
1:B:525:LEU:HD12	1:B:526:PRO:HD2	1.93	0.51
1:A:795:VAL:CG1	1:A:796:ASN:N	2.73	0.51
1:B:550:LYS:O	1:B:554:GLN:HG3	2.11	0.51
1:C:617:THR:HG21	1:C:623:ARG:HA	1.92	0.51
1:A:511:THR:HG22	1:A:512:VAL:N	2.22	0.50
1:C:744:LEU:CD1	1:D:744:LEU:CD1	2.74	0.50
1:D:522:SER:HB3	1:D:525:LEU:HB2	1.94	0.50
1:D:711:MET:HB3	1:D:712:PRO:HD3	1.92	0.50
1:C:518:ASN:HB2	1:C:794:GLN:NE2	2.27	0.50
1:A:525:LEU:HD13	1:A:782:PHE:CZ	2.47	0.50
1:A:603:ASN:O	1:A:607:ILE:HG13	2.12	0.50
1:C:635:VAL:CG2	1:C:679:LEU:CD2	2.87	0.50
1:B:797:GLN:HB2	4:B:917:HOH:O	2.11	0.49
1:D:619:THR:CG2	1:D:622[B]:ASP:HB3	2.42	0.49
1:C:511:THR:CG2	1:C:593:GLN:HE22	2.25	0.49
1:D:586:ILE:O	1:D:595:ARG:NH1	2.46	0.49
1:C:805:ASN:HD22	1:C:805:ASN:C	2.21	0.49
1:C:729:MET:HE2	1:C:729:MET:CA	2.25	0.49
1:A:658:GLN:H	1:A:658:GLN:NE2	2.06	0.49
1:B:607:ILE:HD11	1:B:724:PHE:CD2	2.48	0.49
1:B:670:ARG:NH2	1:B:678:ILE:HG12	2.24	0.49
1:D:698:THR:HG23	1:D:698:THR:O	2.11	0.49
1:A:736:SER:OG	1:A:739:ILE:HD12	2.12	0.49
1:B:732:LYS:HG2	1:B:733:ASN:ND2	2.28	0.49
1:A:713:LEU:O	1:A:717:MET:HG3	2.12	0.48
1:B:732:LYS:HG2	1:B:733:ASN:N	2.28	0.48
1:B:512:VAL:CG2	1:B:513:SER:N	2.77	0.48
1:B:670:ARG:NH2	4:B:923:HOH:O	2.46	0.48
1:B:795:VAL:HG12	1:B:796:ASN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:LEU:HD12	1:C:808:LEU:HD22	1.95	0.48
1:D:559:MET:HE2	1:D:779:LYS:HA	1.95	0.48
1:A:774:MET:HB2	1:A:774:MET:HE2	1.79	0.48
1:D:788:TRP:CE2	1:D:800:ARG:HB3	2.48	0.48
1:C:661:ARG:HH22	1:C:813:ARG:HA	1.76	0.48
1:A:802:GLU:HA	1:A:802:GLU:OE1	2.13	0.47
1:B:586:ILE:CG2	1:B:594:LEU:HD13	2.44	0.47
1:C:566:ILE:HD11	1:C:583:LEU:HD21	1.96	0.47
1:A:736:SER:OG	1:A:739:ILE:CD1	2.62	0.47
1:C:603:ASN:HD21	1:C:723:THR:HA	1.79	0.47
1:B:529:ASN:HD21	1:B:785:ARG:HE	1.62	0.47
1:B:745:ALA:HB3	2:B:834:POG:C16	2.44	0.47
1:A:731:GLU:O	1:A:732:LYS:C	2.57	0.47
1:B:795:VAL:CG1	1:B:796:ASN:N	2.77	0.47
1:C:548:ASP:OD1	1:C:548:ASP:C	2.57	0.47
1:B:539:ARG:HD2	1:B:539:ARG:C	2.37	0.47
1:A:739:ILE:HD12	1:A:739:ILE:N	2.30	0.47
1:B:661:ARG:NH2	1:B:816:GLU:O	2.47	0.47
1:C:524:PHE:HE2	1:C:772:GLU:HG2	1.79	0.47
1:A:557:LEU:HD22	1:A:641:MET:HB3	1.96	0.46
1:B:614:LEU:CD2	1:B:662:LEU:HD11	2.44	0.46
1:D:529:ASN:HB3	1:D:790:SER:HB3	1.97	0.46
1:B:613:ILE:HD11	1:B:630:ILE:CD1	2.45	0.46
1:B:613:ILE:HD11	1:B:630:ILE:HD12	1.96	0.46
1:D:559:MET:HE3	4:D:928:HOH:O	2.14	0.46
1:A:562:ARG:HH22	1:A:775:ASN:HD21	1.64	0.46
1:B:536:LEU:HB3	1:B:786:LEU:HD11	1.97	0.46
1:B:593:GLN:HE21	1:B:593:GLN:HA	1.81	0.46
1:A:661:ARG:NH2	1:A:816:GLU:O	2.48	0.46
1:C:667:THR:HG23	1:C:671:HIS:HE1	1.80	0.46
1:B:627:LEU:HD11	1:B:654:LEU:HD22	1.98	0.46
1:B:732:LYS:HD3	1:B:733:ASN:ND2	2.31	0.46
1:C:729:MET:O	1:C:731:GLU:HG2	2.15	0.46
1:D:690:LEU:O	1:D:695:ARG:HG2	2.16	0.46
1:B:701:PRO:HB2	4:B:500:HOH:O	2.16	0.46
1:C:655:GLU:HG3	4:C:839:HOH:O	2.15	0.46
1:D:657:PRO:HD2	1:D:725:GLU:OE1	2.16	0.46
1:B:577:MET:HE3	1:B:579:VAL:O	2.17	0.45
1:D:511:THR:CG2	1:D:512:VAL:H	2.21	0.45
1:A:711:MET:HB3	1:A:712:PRO:HD3	1.98	0.45
1:D:689:LYS:HD3	4:D:921:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:PRO:HA	1:B:660:THR:CG2	2.41	0.45
1:D:599:ILE:HD11	1:D:714:VAL:CG1	2.46	0.45
1:D:628:SER:O	1:D:632:GLN:HG3	2.17	0.45
1:C:706:SER:HB3	1:C:761:ALA:HB2	1.98	0.45
1:A:544:PHE:CZ	1:A:629:LYS:HG3	2.52	0.45
1:A:590:HIS:H	1:A:590:HIS:HD2	1.62	0.45
1:B:708:PRO:HG2	1:B:710:LEU:HD21	1.97	0.45
1:A:524:PHE:CE2	1:A:772:GLU:HG2	2.50	0.45
1:A:516:ARG:HA	1:A:517:PRO:HD2	1.80	0.44
1:A:530:LYS:HE2	1:A:530:LYS:HB3	1.76	0.44
1:A:555:HIS:CD2	1:A:774:MET:CG	3.00	0.44
1:A:572:GLU:O	1:A:576:ASN:HB2	2.17	0.44
1:B:564:ALA:O	1:B:582:GLY:HA3	2.17	0.44
1:D:523:LYS:CE	1:D:772:GLU:OE1	2.65	0.44
1:D:541:LYS:HE2	1:D:616:CYS:O	2.16	0.44
1:A:586:ILE:HG23	1:A:594:LEU:HD13	1.99	0.44
1:A:591:GLY:HA2	4:A:844:HOH:O	2.16	0.44
1:A:670:ARG:NH2	4:A:905:HOH:O	2.50	0.44
1:C:680:TYR:HA	1:C:684:LEU:HB2	1.99	0.44
1:D:599:ILE:HD11	1:D:714:VAL:HG12	1.99	0.44
1:B:599:ILE:HD11	1:B:714:VAL:HG12	1.98	0.44
4:B:868:HOH:O	1:D:756:SER:HB3	2.18	0.44
1:B:640:SER:C	1:B:641:MET:HE2	2.43	0.44
1:B:745:ALA:CB	2:B:834:POG:C16	2.96	0.44
1:A:555:HIS:CD2	1:A:774:MET:HG2	2.54	0.43
1:B:518:ASN:HD21	1:B:791:LYS:HA	1.83	0.43
1:D:534:THR:HG23	1:D:535:ALA:N	2.33	0.43
1:D:689:LYS:HE3	1:D:693:GLU:OE2	2.18	0.43
2:B:834:POG:H183	1:D:697:SER:CB	2.48	0.43
1:A:817:PRO:HA	1:A:818:PRO:HD3	1.89	0.43
1:C:539:ARG:O	1:C:542:GLU:HB2	2.18	0.43
1:C:586:ILE:O	1:C:595:ARG:NH1	2.48	0.43
1:A:700:VAL:HA	1:A:701:PRO:HD3	1.85	0.43
1:A:530:LYS:CG	1:A:533:GLU:CG	2.95	0.43
1:B:592:HIS:HA	1:B:595:ARG:NH2	2.34	0.43
1:B:729:MET:HE2	1:B:729:MET:HA	2.01	0.43
1:B:696:GLU:HB3	4:B:836:HOH:O	2.18	0.43
1:B:700:VAL:HA	1:B:701:PRO:HD3	1.81	0.43
1:C:523:LYS:HE3	1:C:772:GLU:OE2	2.19	0.42
1:D:780:THR:O	1:D:784:MET:HG3	2.19	0.42
1:A:573:MET:O	1:A:577:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ARG:HH21	1:B:773:GLU:CD	2.27	0.42
1:B:745:ALA:HB3	2:B:834:POG:H162	2.01	0.42
1:C:776:GLU:OE2	1:C:779:LYS:HE3	2.19	0.42
1:D:524:PHE:CD1	1:D:773:GLU:HG3	2.54	0.42
1:D:713:LEU:HD22	1:D:747:ALA:HB2	2.01	0.42
1:C:648:SER:HA	4:C:869:HOH:O	2.18	0.42
1:A:555:HIS:CG	1:A:774:MET:CG	3.03	0.42
1:A:803:LYS:NZ	4:A:862:HOH:O	2.52	0.42
1:C:530:LYS:HB2	1:C:530:LYS:HE2	1.58	0.42
1:B:529:ASN:ND2	1:B:785:ARG:NH2	2.53	0.42
1:B:558:SER:O	1:B:562:ARG:HD3	2.19	0.42
1:C:557:LEU:HD22	1:C:641:MET:HB3	2.01	0.42
1:A:690:LEU:HD23	1:A:690:LEU:HA	1.63	0.42
1:A:737:CYS:HA	1:A:740:MET:HE3	2.02	0.42
2:B:834:POG:H173	2:B:834:POG:H152	1.75	0.42
1:C:683:GLN:HA	1:C:683:GLN:NE2	2.22	0.42
1:D:594:LEU:HD23	1:D:594:LEU:HA	1.79	0.42
1:D:795:VAL:CG1	1:D:796:ASN:N	2.81	0.42
1:A:789:GLY:O	1:A:793:ALA:HB2	2.20	0.41
1:C:605:MET:O	1:C:609:ILE:HG12	2.20	0.41
1:A:533:GLU:O	1:A:537:LEU:HG	2.20	0.41
1:A:631:ILE:HD13	1:A:680:TYR:HB2	2.01	0.41
1:C:717:MET:HE2	1:C:717:MET:HB3	1.93	0.41
1:D:526:PRO:HA	1:D:527:PRO:HD2	1.71	0.41
1:D:543:LEU:HD21	1:D:774:MET:HA	2.02	0.41
1:D:803:LYS:O	1:D:807:ILE:HG13	2.20	0.41
1:C:511:THR:OG1	1:C:512:VAL:N	2.53	0.41
1:C:526:PRO:O	1:C:529:ASN:HB3	2.20	0.41
1:A:585:LEU:HD23	1:A:594:LEU:HD12	2.02	0.41
1:B:681:GLU:HG2	4:B:859:HOH:O	2.20	0.41
1:C:511:THR:HG23	1:C:512:VAL:O	2.20	0.41
1:D:599:ILE:HG13	1:D:714:VAL:CG1	2.50	0.41
1:A:683:GLN:C	1:A:686:PRO:HD2	2.45	0.41
1:B:523:LYS:HE3	1:B:772:GLU:OE2	2.20	0.41
1:B:511:THR:HG21	4:B:894:HOH:O	2.19	0.41
1:C:536:LEU:HB3	1:C:786:LEU:HD21	2.01	0.41
1:C:543:LEU:HD23	1:C:543:LEU:HA	1.85	0.41
1:C:780:THR:O	1:C:784:MET:HG3	2.20	0.41
1:D:692:HIS:CD2	4:D:908:HOH:O	2.64	0.41
1:B:620:LEU:HD11	1:B:665:THR:HA	2.03	0.41
1:B:669:LEU:HG	1:B:677:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:LYS:HD2	1:B:814:LYS:HA	1.88	0.41
1:C:701:PRO:HB2	4:C:834:HOH:O	2.21	0.41
1:D:619:THR:HG23	1:D:622[B]:ASP:HB3	2.03	0.41
1:A:595:ARG:HG2	1:A:714:VAL:HG22	2.03	0.41
1:B:652:LYS:CE	1:B:727:THR:OG1	2.66	0.41
1:B:683:GLN:C	1:B:686:PRO:HD2	2.46	0.41
1:B:748:ARG:HH11	1:B:748:ARG:CB	2.33	0.41
1:B:786:LEU:HD12	1:B:786:LEU:HA	1.94	0.41
1:D:595:ARG:HG2	1:D:714:VAL:HG22	2.03	0.41
1:D:708:PRO:HB3	4:D:852:HOH:O	2.20	0.41
1:B:594:LEU:HD23	1:B:594:LEU:HA	1.95	0.41
1:C:728:ASP:O	1:C:729:MET:HE2	2.21	0.41
1:D:523:LYS:HE3	1:D:772:GLU:CD	2.45	0.41
1:A:574:ARG:CZ	1:A:574:ARG:CB	3.00	0.40
1:B:614:LEU:HD11	1:B:659:ILE:HD13	2.03	0.40
1:B:658:GLN:HE21	1:B:658:GLN:N	2.07	0.40
1:B:732:LYS:HD3	1:B:733:ASN:HD22	1.86	0.40
1:B:617:THR:HG21	1:B:623:ARG:HA	2.02	0.40
1:A:560:ASP:OD2	1:A:643:ASP:OD2	2.39	0.40
1:B:652:LYS:HE3	1:B:727:THR:HG21	2.03	0.40
1:D:619:THR:HG22	1:D:622[B]:ASP:HB3	2.02	0.40
1:A:715:THR:CG2	1:A:730:TRP:CD1	3.04	0.40
1:A:740:MET:HE3	1:A:740:MET:HB2	1.88	0.40
1:A:782:PHE:CD2	1:A:782:PHE:C	2.99	0.40
1:B:715:THR:HG21	1:B:728:ASP:HB3	2.02	0.40
1:C:586:ILE:CG2	1:C:594:LEU:HD13	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/333 (92%)	292 (95%)	14 (5%)	1 (0%)	36	50
1	B	309/333 (93%)	295 (96%)	14 (4%)	0	100	100
1	C	307/333 (92%)	291 (95%)	15 (5%)	1 (0%)	36	50
1	D	308/333 (92%)	293 (95%)	14 (4%)	1 (0%)	36	50
All	All	1231/1332 (92%)	1171 (95%)	57 (5%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	616	CYS
1	A	732	LYS
1	C	615	GLY

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	273/295 (92%)	258 (94%)	15 (6%)	19	34
1	B	275/295 (93%)	250 (91%)	25 (9%)	9	14
1	C	273/295 (92%)	256 (94%)	17 (6%)	16	29
1	D	274/295 (93%)	253 (92%)	21 (8%)	12	20
All	All	1095/1180 (93%)	1017 (93%)	78 (7%)	14	23

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	THR
1	A	544	PHE
1	A	590	HIS
1	A	593	GLN
1	A	594	LEU
1	A	658	GLN
1	A	660	THR
1	A	684	LEU

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Mol	Chain	Res	Type
1	A	715	THR
1	A	720	GLN
1	A	741	LEU
1	A	758	ARG
1	A	759	MET
1	A	762	GLU
1	A	769	GLN
1	B	513	SER
1	B	523	LYS
1	B	534	THR
1	B	590	HIS
1	B	593	GLN
1	B	594	LEU
1	B	629	LYS
1	B	658	GLN
1	B	670	ARG
1	B	675[A]	GLN
1	B	675[B]	GLN
1	B	683	GLN
1	B	684	LEU
1	B	700	VAL
1	B	714	VAL
1	B	720	GLN
1	B	736	SER
1	B	741	LEU
1	B	748	ARG
1	B	771	ASP
1	B	777	ILE
1	B	781[A]	GLU
1	B	781[B]	GLU
1	B	798	THR
1	B	809	THR
1	C	530	LYS
1	C	534	THR
1	C	548	ASP
1	C	594	LEU
1	C	617	THR
1	C	629	LYS
1	C	660	THR
1	C	679	LEU
1	C	683	GLN
1	C	700	VAL

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Mol	Chain	Res	Type
1	C	715	THR
1	C	731	GLU
1	C	736	SER
1	C	741	LEU
1	C	769	GLN
1	C	786	LEU
1	C	794	GLN
1	D	539	ARG
1	D	548	ASP
1	D	594	LEU
1	D	609	ILE
1	D	617	THR
1	D	629	LYS
1	D	658	GLN
1	D	661	ARG
1	D	683	GLN
1	D	684	LEU
1	D	698	THR
1	D	700	VAL
1	D	711	MET
1	D	714	VAL
1	D	723	THR
1	D	759	MET
1	D	777	ILE
1	D	781[A]	GLU
1	D	781[B]	GLU
1	D	794	GLN
1	D	813	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
1	A	529	ASN
1	A	547	ASN
1	A	590	HIS
1	A	593	GLN
1	A	658	GLN
1	A	671	HIS
1	A	675	GLN
1	A	683	GLN
1	A	704	ASN

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Mol	Chain	Res	Type
1	A	775	ASN
1	A	794	GLN
1	A	805	ASN
1	B	518	ASN
1	B	529	ASN
1	B	547	ASN
1	B	590	HIS
1	B	593	GLN
1	B	658	GLN
1	B	683	GLN
1	B	733	ASN
1	B	775	ASN
1	B	797	GLN
1	C	518	ASN
1	C	593	GLN
1	C	632	GLN
1	C	672	GLN
1	C	675	GLN
1	C	683	GLN
1	C	704	ASN
1	C	775	ASN
1	C	794	GLN
1	C	805	ASN
1	D	554	GLN
1	D	632	GLN
1	D	658	GLN
1	D	675	GLN
1	D	683	GLN
1	D	692	HIS
1	D	775	ASN
1	D	794	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are unknown - leaving 2 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	POG	B	834	-	16,16,28	1.73	6 (37%)	19,19,34	2.05	6 (31%)
2	POG	A	834	-	15,15,28	1.42	2 (13%)	17,17,34	2.35	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POG	B	834	-	-	7/17/17/32	-
2	POG	A	834	-	-	8/16/16/32	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	834	POG	O6-C12	-3.09	1.39	1.44
2	A	834	POG	O5-C10	-3.08	1.39	1.44
2	B	834	POG	O5-C10	-2.91	1.39	1.44
2	B	834	POG	O7-C14	-2.69	1.39	1.44
2	B	834	POG	C9-C10	2.42	1.55	1.51
2	A	834	POG	O6-C12	-2.35	1.40	1.44
2	B	834	POG	C13-C14	2.19	1.55	1.50
2	B	834	POG	O5-C11	-2.02	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	834	POG	C11-O5-C10	5.48	123.14	115.05
2	B	834	POG	O4-C9-C10	4.17	122.49	111.77
2	B	834	POG	O7-C15-C5	3.83	116.40	108.94
2	A	834	POG	C9-O4-C8	3.52	120.24	115.05
2	A	834	POG	O5-C11-C12	3.35	118.98	110.82
2	B	834	POG	C11-O5-C10	3.20	119.78	115.05
2	B	834	POG	O6-C13-C14	2.99	118.10	110.82
2	A	834	POG	O4-C9-C10	2.88	117.82	110.82
2	B	834	POG	O5-C11-C12	2.86	117.77	110.82
2	A	834	POG	O6-C13-C14	2.76	118.67	110.68
2	A	834	POG	O3-C7-C8	2.61	118.48	111.77
2	B	834	POG	O5-C10-C9	2.53	115.38	108.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	834	POG	O3-C7-C8-O4
2	A	834	POG	C20-C8-O4-C9
2	A	834	POG	C19-C10-C9-O4
2	B	834	POG	O5-C11-C12-O6
2	B	834	POG	O6-C13-C14-C17
2	B	834	POG	C17-C14-O7-C15
2	A	834	POG	O6-C13-C14-C17
2	A	834	POG	C12-C11-O5-C10
2	B	834	POG	O5-C11-C12-C18
2	A	834	POG	O5-C10-C9-O4
2	B	834	POG	O6-C13-C14-O7
2	A	834	POG	C14-C13-O6-C12
2	B	834	POG	O7-C15-C5-C16
2	A	834	POG	O3-C7-C8-C20
2	B	834	POG	C5-C15-O7-C14

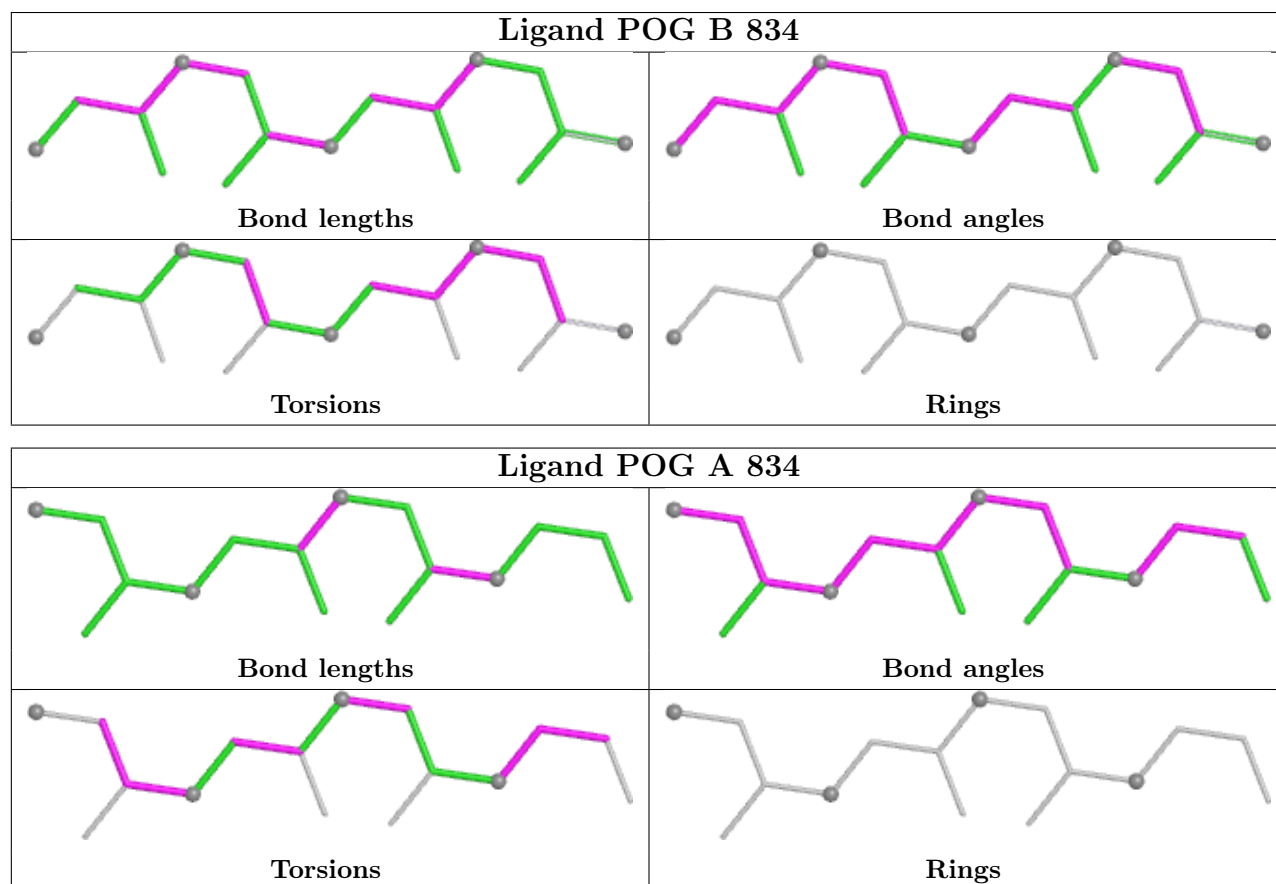
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	834	POG	7	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	308/333 (92%)	-0.65	1 (0%) 90 88	16, 37, 80, 125	1 (0%)
1	B	308/333 (92%)	-0.59	4 (1%) 75 71	15, 37, 76, 125	3 (0%)
1	C	308/333 (92%)	-0.65	2 (0%) 85 83	17, 37, 69, 129	1 (0%)
1	D	308/333 (92%)	-0.60	3 (0%) 79 76	16, 39, 75, 123	2 (0%)
All	All	1232/1332 (92%)	-0.62	10 (0%) 82 80	15, 37, 76, 129	7 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	511	THR	4.2
1	C	511	THR	3.6
1	B	733	ASN	3.4
1	D	512	VAL	2.6
1	B	512	VAL	2.6
1	A	512	VAL	2.4
1	B	616	CYS	2.2
1	B	732	LYS	2.2
1	C	616	CYS	2.2
1	D	794	GLN	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](#)

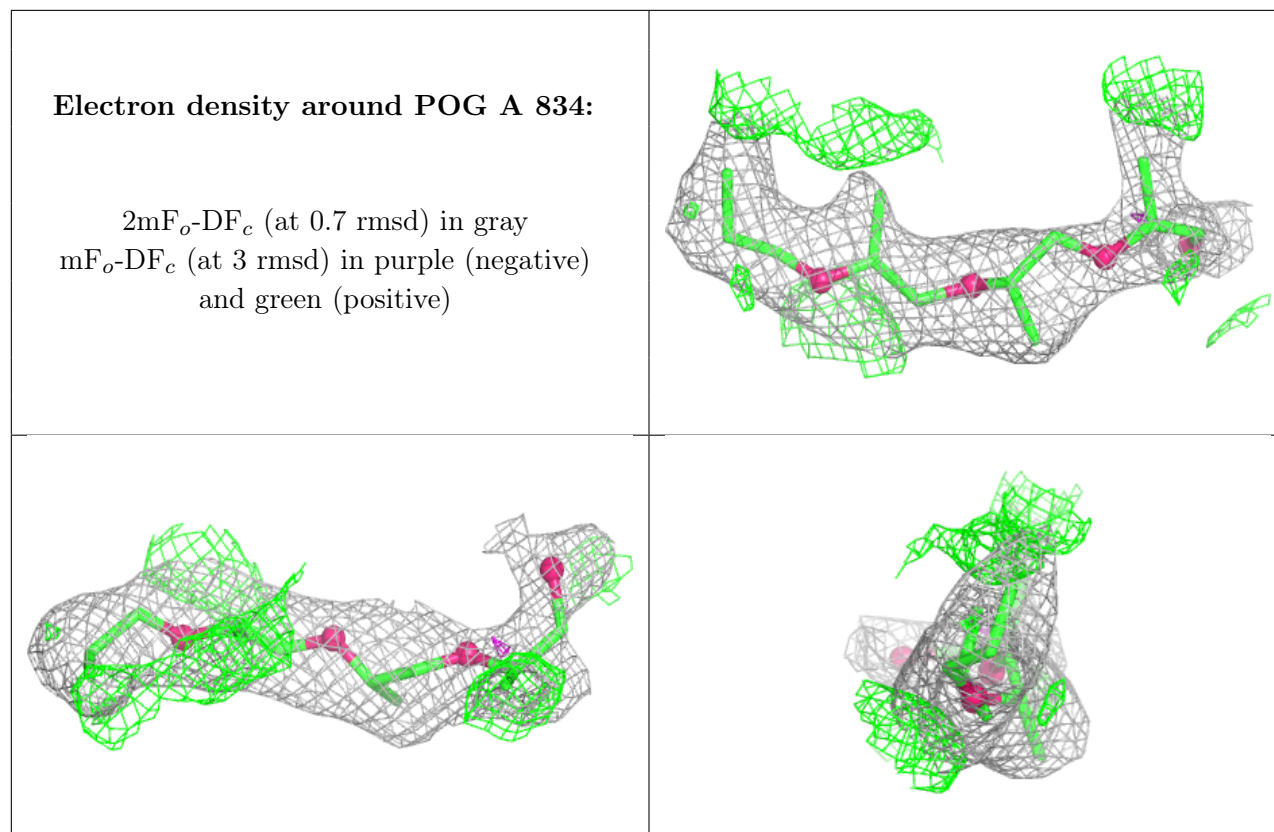
There are no oligosaccharides in this entry.

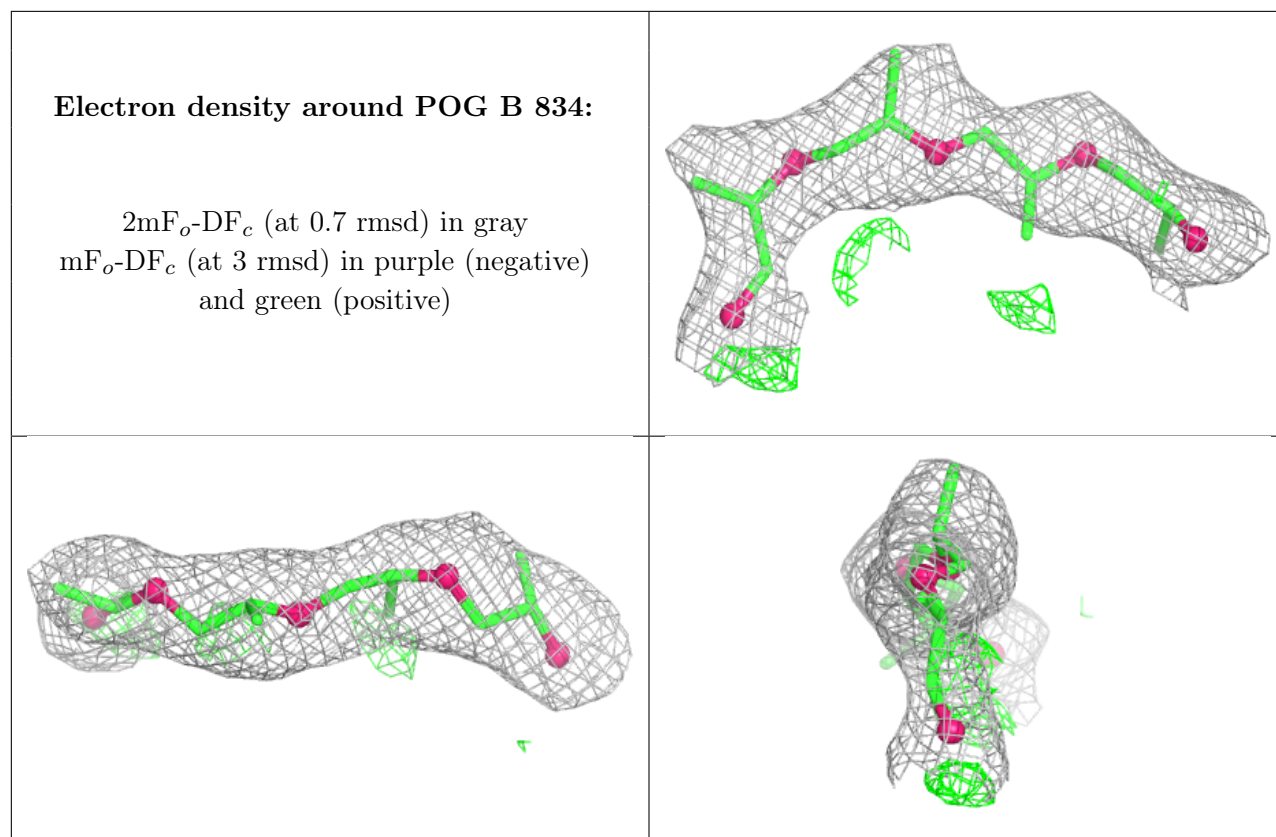
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	POG	A	834	16/29	0.83	0.14	23,54,74,75	0
3	UNX	D	834	1/1	0.86	0.21	51,51,51,51	0
3	UNX	D	836	1/1	0.86	0.18	39,39,39,39	0
3	UNX	D	837	1/1	0.87	0.24	43,43,43,43	0
3	UNX	D	835	1/1	0.88	0.24	42,42,42,42	0
2	POG	B	834	17/29	0.91	0.11	37,54,64,67	0
3	UNX	D	838	1/1	0.91	0.18	35,35,35,35	0
3	UNX	D	841	1/1	0.91	0.17	47,47,47,47	0
3	UNX	D	840	1/1	0.93	0.26	41,41,41,41	0
3	UNX	D	839	1/1	0.93	0.14	33,33,33,33	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.