



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:14 PM UTC

PDB ID : 4CBY / pdb_00004cby
Title : Design, synthesis, and biological evaluation of potent and selective Class IIa HDAC inhibitors as a potential therapy for Huntington's disease
Authors : Burli, R.W.; Luckhurst, C.A.; Aziz, O.; Matthews, K.L.; Yates, D.; Lyons, K.A.; Beconi, M.; McAllister, G.; Breccia, P.; Stott, A.J.; Penrose, S.D.; Wall, M.; Lamers, M.; Leonard, P.; Mueller, I.; Richardson, C.M.; Jarvis, R.; Stones, L.; Hughes, S.; Wishart, G.; Haughan, A.F.; O'Connell, C.; Mead, T.; McNeil, H.; Vann, J.; Mangette, J.; Maillard, M.; Beaumont, V.; Munoz-Sanjuan, I.; Dominguez, C.
Deposited on : 2013-10-17
Resolution : 2.72 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)

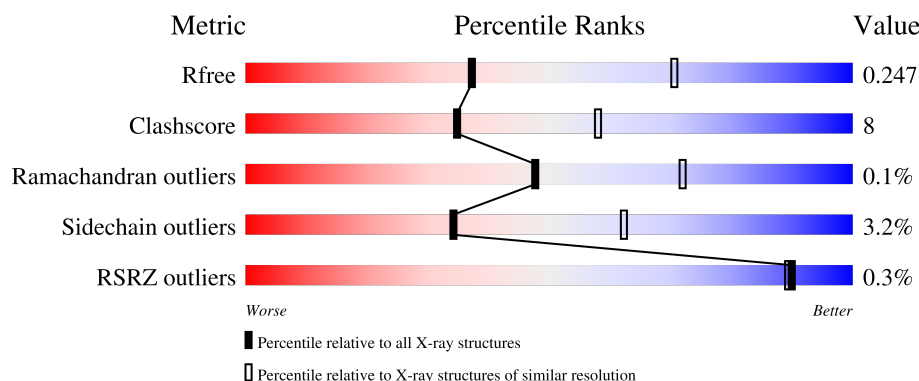
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	395	
1	B	395	

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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

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Mol	Chain	Length	Quality of chain
1	C	395	% 79% 16%
1	D	395	83% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11435 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 HISTONE DEACETYLASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2823	1782	494	527	20			
1	B	380	Total	C	N	O	S	0	0	0
			2795	1767	483	525	20			
1	C	380	Total	C	N	O	S	0	0	0
			2802	1764	488	530	20			
1	D	383	Total	C	N	O	S	0	0	0
			2812	1772	492	528	20			

There are 40 discrepancies between the modelled and reference sequences:

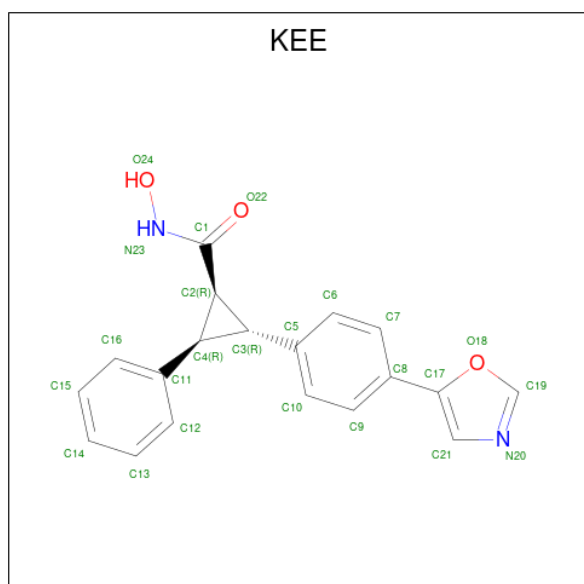
Chain	Residue	Modelled	Actual	Comment	Reference
A	645	MET	-	expression tag	UNP P56524
A	646	GLY	-	expression tag	UNP P56524
A	647	SER	-	expression tag	UNP P56524
A	728	ALA	LEU	engineered mutation	UNP P56524
A	1034	HIS	-	expression tag	UNP P56524
A	1035	HIS	-	expression tag	UNP P56524
A	1036	HIS	-	expression tag	UNP P56524
A	1037	HIS	-	expression tag	UNP P56524
A	1038	HIS	-	expression tag	UNP P56524
A	1039	HIS	-	expression tag	UNP P56524
B	645	MET	-	expression tag	UNP P56524
B	646	GLY	-	expression tag	UNP P56524
B	647	SER	-	expression tag	UNP P56524
B	728	ALA	LEU	engineered mutation	UNP P56524
B	1034	HIS	-	expression tag	UNP P56524
B	1035	HIS	-	expression tag	UNP P56524
B	1036	HIS	-	expression tag	UNP P56524
B	1037	HIS	-	expression tag	UNP P56524
B	1038	HIS	-	expression tag	UNP P56524
B	1039	HIS	-	expression tag	UNP P56524
C	645	MET	-	expression tag	UNP P56524

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Chain	Residue	Modelled	Actual	Comment	Reference
C	646	GLY	-	expression tag	UNP P56524
C	647	SER	-	expression tag	UNP P56524
C	728	ALA	LEU	engineered mutation	UNP P56524
C	1034	HIS	-	expression tag	UNP P56524
C	1035	HIS	-	expression tag	UNP P56524
C	1036	HIS	-	expression tag	UNP P56524
C	1037	HIS	-	expression tag	UNP P56524
C	1038	HIS	-	expression tag	UNP P56524
C	1039	HIS	-	expression tag	UNP P56524
D	645	MET	-	expression tag	UNP P56524
D	646	GLY	-	expression tag	UNP P56524
D	647	SER	-	expression tag	UNP P56524
D	728	ALA	LEU	engineered mutation	UNP P56524
D	1034	HIS	-	expression tag	UNP P56524
D	1035	HIS	-	expression tag	UNP P56524
D	1036	HIS	-	expression tag	UNP P56524
D	1037	HIS	-	expression tag	UNP P56524
D	1038	HIS	-	expression tag	UNP P56524
D	1039	HIS	-	expression tag	UNP P56524

- Molecule 2 is (1R,2R,3R)-2-[4-(1,3-oxazol-5-yl)phenyl]-N-oxidanyl-3-phenyl-cyclopropane-1-carboxamide (CCD ID: KEE) (formula: C₁₉H₁₆N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	19	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			24	19	2	3		
2	C	1	Total	C	N	O	0	0
			24	19	2	3		
2	D	1	Total	C	N	O	0	0
			24	19	2	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		
4	C	2	Total	Na	0	0
			2	2		
4	D	2	Total	Na	0	0
			2	2		

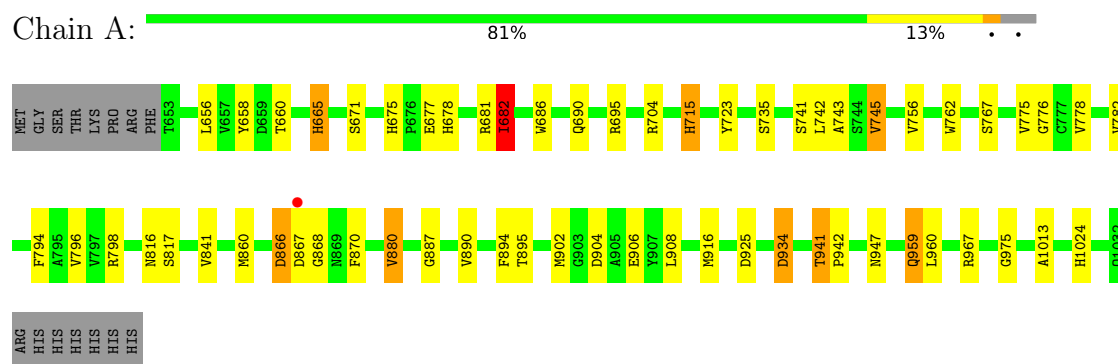
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	23	Total	O	0	0
			23	23		
5	C	24	Total	O	0	0
			24	24		
5	D	22	Total	O	0	0
			22	22		

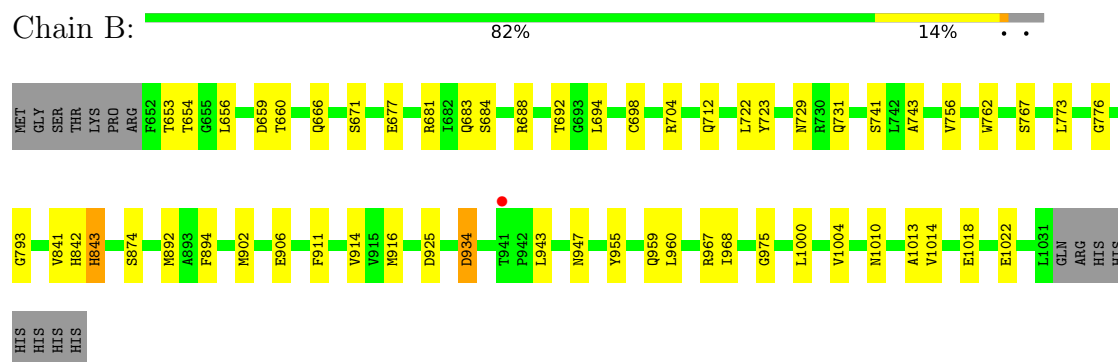
3 Residue-property plots

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.

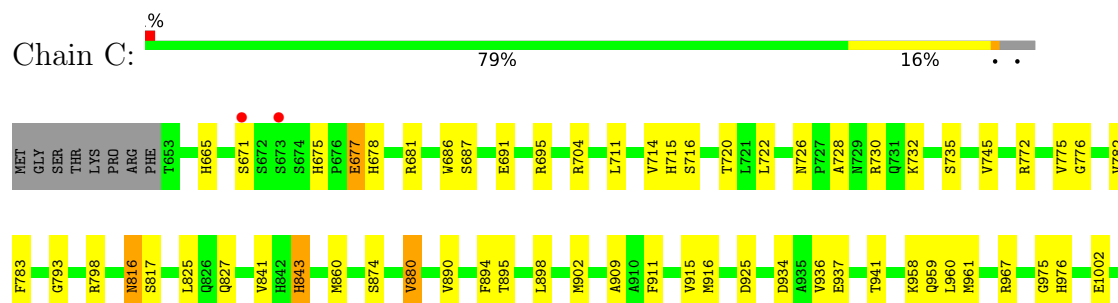
• Molecule 1: HISTONE DEACETYLASE 4



• Molecule 1: HISTONE DEACETYLASE 4

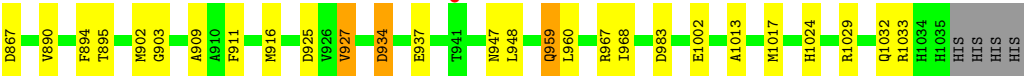
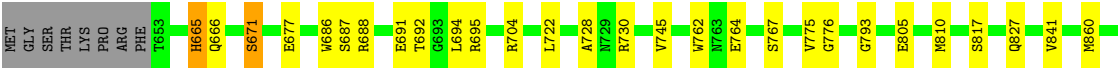
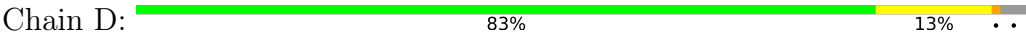


• Molecule 1: HISTONE DEACETYLASE 4





● Molecule 1: HISTONE DEACETYLASE 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.15Å 161.82Å 83.73Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	83.10 – 2.72 83.10 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.3 (83.10-2.72) 98.4 (83.10-2.72)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.246 0.212 , 0.247	Depositor DCC
R_{free} test set	1886 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11435	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 37.36 % 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 4.3423e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NA, KEE

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	0.82	4/2887 (0.1%)	0.90	11/3924 (0.3%)
1	B	0.84	8/2860 (0.3%)	0.84	4/3894 (0.1%)
1	C	0.84	4/2865 (0.1%)	0.90	11/3899 (0.3%)
1	D	0.82	3/2876 (0.1%)	0.87	5/3912 (0.1%)
All	All	0.83	19/11488 (0.2%)	0.88	31/15629 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	712	GLN	CD-NE2	-6.65	1.19	1.33
1	C	816	ASN	CG-OD1	6.24	1.35	1.23
1	B	947	ASN	CG-OD1	5.96	1.34	1.23
1	B	959	GLN	CD-OE1	5.69	1.34	1.23
1	C	1007	GLN	CD-OE1	5.69	1.34	1.23
1	D	827	GLN	CD-OE1	5.64	1.34	1.23
1	A	959	GLN	CD-OE1	5.56	1.34	1.23
1	C	726	ASN	CG-OD1	5.54	1.34	1.23
1	D	959	GLN	CD-NE2	-5.53	1.21	1.33
1	B	729	ASN	CG-OD1	5.41	1.33	1.23
1	B	683	GLN	CD-OE1	5.38	1.33	1.23
1	D	947	ASN	CG-OD1	5.35	1.33	1.23
1	C	675	HIS	ND1-CE1	5.26	1.37	1.32
1	A	690	GLN	CD-NE2	-5.21	1.22	1.33
1	B	842	HIS	CG-ND1	-5.16	1.32	1.38
1	A	690	GLN	CD-OE1	5.15	1.33	1.23
1	B	712	GLN	CD-OE1	5.14	1.33	1.23
1	A	675	HIS	CG-ND1	-5.09	1.32	1.38
1	B	959	GLN	CD-NE2	-5.03	1.22	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	682	ILE	CB-CA-C	-8.42	100.96	112.24
1	A	870	PHE	N-CA-C	-7.05	100.05	110.48
1	B	843	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	A	678	HIS	CB-CG-CD2	-6.92	122.20	131.20
1	A	868	GLY	N-CA-C	6.92	124.87	115.32
1	C	715	HIS	CB-CG-CD2	-6.91	122.22	131.20
1	C	678	HIS	CB-CG-CD2	-6.90	122.23	131.20
1	C	976	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	C	843	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	A	715	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	D	1024	HIS	CB-CG-CD2	-6.43	122.83	131.20
1	D	665	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	665	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	B	843	HIS	CB-CG-ND1	5.87	131.50	122.70
1	C	793	GLY	N-CA-C	5.78	119.20	110.18
1	B	731	GLN	N-CA-CB	5.75	118.76	110.20
1	C	715	HIS	CB-CG-ND1	5.73	131.30	122.70
1	C	678	HIS	CB-CG-ND1	5.67	131.21	122.70
1	C	843	HIS	CB-CG-ND1	5.67	131.20	122.70
1	C	976	HIS	CB-CG-ND1	5.60	131.09	122.70
1	A	678	HIS	CB-CG-ND1	5.57	131.05	122.70
1	A	715	HIS	CB-CG-ND1	5.50	130.95	122.70
1	D	665	HIS	CB-CG-ND1	5.48	130.92	122.70
1	B	793	GLY	N-CA-C	5.42	119.55	110.56
1	C	880	VAL	N-CA-CB	-5.39	105.91	112.33
1	A	866	ASP	CA-C-N	-5.33	114.67	122.40
1	A	866	ASP	C-N-CA	-5.33	114.67	122.40
1	C	714	VAL	CB-CA-C	-5.26	106.25	111.30
1	D	793	GLY	N-CA-C	5.07	118.97	110.56
1	A	665	HIS	CB-CG-ND1	5.05	130.27	122.70
1	D	1024	HIS	CB-CG-ND1	5.03	130.25	122.70

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	2823	0	2753	46	0
1	B	2795	0	2683	44	0
1	C	2802	0	2693	44	0
1	D	2812	0	2701	40	0
2	A	24	0	13	0	0
2	B	24	0	12	0	0
2	C	24	0	13	0	0
2	D	24	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	22	0	0	1	0
5	B	23	0	0	2	0
5	C	24	0	0	1	0
5	D	22	0	0	4	0
All	All	11435	0	10881	167	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 8.

All (167) 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:916:MET:HE1	1:B:960:LEU:HD23	1.32	1.12
1:D:688:ARG:NH2	1:D:983:ASP:OD1	1.96	0.98
1:B:902:MET:HE1	1:B:1013:ALA:HB2	1.47	0.96
1:A:902:MET:HE1	1:A:1013:ALA:HB2	1.46	0.94
1:D:937:GLU:CB	5:D:2017:HOH:O	2.16	0.94
1:A:682:ILE:HG23	1:A:796:VAL:HG12	1.52	0.92
1:B:892:MET:HE1	1:B:914:VAL:HG21	1.55	0.89
1:C:860:MET:HE3	1:C:890:VAL:HG11	1.54	0.88
1:B:968:ILE:HB	5:B:2019:HOH:O	1.76	0.86
1:C:894:PHE:CD1	1:C:902:MET:HE2	2.11	0.85
1:A:916:MET:HE3	1:A:959:GLN:HB3	1.56	0.84
1:D:902:MET:HE1	1:D:1013:ALA:HB2	1.58	0.84
1:D:860:MET:HE3	1:D:890:VAL:HG11	1.60	0.83
1:B:916:MET:CE	1:B:960:LEU:HD23	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:958:LYS:HA	1:C:961:MET:HE2	1.62	0.82
1:B:660:THR:CG2	1:D:867:ASP:HB3	2.11	0.80
1:D:894:PHE:CD1	1:D:902:MET:HE2	2.17	0.79
1:C:916:MET:HE1	1:C:960:LEU:HD23	1.64	0.79
1:A:682:ILE:CG2	1:A:796:VAL:HG12	2.13	0.78
1:A:715:HIS:HE1	1:A:816:ASN:H	1.28	0.78
1:A:682:ILE:HD11	1:A:798:ARG:HB2	1.66	0.78
1:B:955:TYR:CE1	1:B:1000:LEU:HD12	2.19	0.78
1:C:902:MET:HE1	1:C:1013:ALA:HB2	1.67	0.77
1:C:665:HIS:O	1:C:798:ARG:NH2	2.17	0.77
1:A:916:MET:HE1	1:A:960:LEU:HD23	1.66	0.77
1:C:677:GLU:OE2	1:C:798:ARG:NH1	2.18	0.76
1:B:892:MET:HE2	1:B:914:VAL:HG11	1.67	0.76
1:A:941:THR:HG23	1:A:942:PRO:HD3	1.67	0.75
1:D:916:MET:HE1	1:D:960:LEU:HD23	1.68	0.75
1:B:902:MET:HE1	1:B:1013:ALA:CB	2.17	0.74
1:A:860:MET:HE2	1:A:890:VAL:HG11	1.68	0.73
1:A:902:MET:HE1	1:A:1013:ALA:CB	2.18	0.73
1:A:916:MET:CE	1:A:960:LEU:HD23	2.18	0.73
1:B:660:THR:HG21	1:D:867:ASP:HB3	1.69	0.72
1:D:902:MET:HE1	1:D:1013:ALA:CB	2.22	0.70
1:B:955:TYR:CE1	1:B:1000:LEU:CD1	2.75	0.69
1:D:909:ALA:HB3	1:D:1017:MET:HE1	1.76	0.68
1:C:860:MET:HE3	1:C:890:VAL:CG1	2.24	0.68
1:D:916:MET:CE	1:D:960:LEU:HD23	2.25	0.66
1:A:902:MET:HE3	1:A:906:GLU:HG2	1.78	0.66
1:B:894:PHE:CD1	1:B:902:MET:HE2	2.32	0.65
1:A:880:VAL:HG22	1:A:1024:HIS:CE1	2.32	0.65
1:B:741:SER:OG	1:B:743:ALA:HB3	1.97	0.64
1:C:902:MET:HE1	1:C:1013:ALA:CB	2.27	0.63
1:C:909:ALA:HB3	1:C:1017:MET:HE1	1.81	0.63
1:C:916:MET:CE	1:C:960:LEU:HD23	2.29	0.62
1:B:892:MET:CE	1:B:914:VAL:HG11	2.29	0.61
1:C:677:GLU:CD	1:C:798:ARG:NH1	2.57	0.61
1:B:955:TYR:CZ	1:B:1000:LEU:CD1	2.83	0.61
1:A:904:ASP:O	1:A:908:LEU:HD12	2.01	0.61
1:A:841:VAL:HG12	1:A:934:ASP:CG	2.25	0.60
1:D:860:MET:HE3	1:D:890:VAL:CG1	2.31	0.60
1:B:660:THR:HG21	1:D:867:ASP:CB	2.31	0.59
1:C:843:HIS:HD2	1:C:874:SER:OG	1.84	0.59
1:B:841:VAL:HG12	1:B:934:ASP:CG	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:MET:HE1	1:A:960:LEU:HA	1.84	0.58
1:A:894:PHE:CD1	1:A:902:MET:HE2	2.40	0.57
1:A:742:LEU:HA	1:A:745:VAL:HG13	1.88	0.56
1:B:660:THR:CG2	1:D:867:ASP:CB	2.83	0.56
1:A:665:HIS:HD2	1:A:767:SER:OG	1.88	0.56
1:C:1010:ASN:O	1:C:1014:VAL:HG23	2.05	0.56
1:A:682:ILE:N	1:A:682:ILE:HD13	2.21	0.55
1:D:860:MET:CE	1:D:890:VAL:HG11	2.34	0.55
1:A:860:MET:HE2	1:A:890:VAL:CG1	2.36	0.55
1:A:941:THR:CG2	1:A:942:PRO:HD3	2.36	0.55
1:B:843:HIS:HD2	1:B:874:SER:OG	1.90	0.55
1:C:916:MET:HE3	1:C:959:GLN:HB3	1.89	0.55
5:B:2006:HOH:O	1:C:1008:ARG:HD3	2.07	0.54
1:D:665:HIS:HD2	1:D:767:SER:OG	1.89	0.54
1:C:898:LEU:HD11	1:C:941:THR:HG23	1.88	0.54
1:B:660:THR:HG21	1:D:867:ASP:CG	2.32	0.54
1:B:943:LEU:HD23	1:B:943:LEU:O	2.07	0.54
1:B:955:TYR:CZ	1:B:1000:LEU:HD12	2.42	0.54
1:D:909:ALA:CB	1:D:1017:MET:HE1	2.37	0.54
1:D:902:MET:CE	1:D:1013:ALA:HB2	2.35	0.54
1:B:653:THR:OG1	1:B:654:THR:N	2.38	0.53
1:D:692:THR:HG23	1:D:694:LEU:H	1.75	0.52
1:B:692:THR:HG23	1:B:694:LEU:H	1.75	0.51
1:D:805:GLU:HG3	1:D:810:MET:HE3	1.91	0.51
1:C:841:VAL:HG12	1:C:934:ASP:CG	2.35	0.51
1:A:741:SER:OG	1:A:743:ALA:HB3	2.11	0.51
1:B:902:MET:HE3	1:B:906:GLU:HG2	1.92	0.51
1:C:677:GLU:CD	1:C:798:ARG:HH11	2.19	0.51
1:A:794:PHE:CE2	1:A:796:VAL:HG22	2.46	0.51
1:B:660:THR:HG23	1:D:867:ASP:HB3	1.92	0.50
1:D:1002:GLU:CB	5:D:2019:HOH:O	2.59	0.50
1:C:909:ALA:CB	1:C:1017:MET:HE1	2.42	0.50
1:B:1010:ASN:O	1:B:1014:VAL:HG23	2.13	0.49
1:C:681:ARG:NH1	1:C:975:GLY:O	2.41	0.49
1:D:775:VAL:HG22	1:D:817:SER:HA	1.95	0.49
1:C:958:LYS:HG2	1:C:961:MET:HE2	1.95	0.48
1:A:681:ARG:NH1	1:A:975:GLY:O	2.44	0.48
1:B:1018:GLU:O	1:B:1022:GLU:HG3	2.13	0.48
1:A:902:MET:CE	1:A:906:GLU:HG2	2.43	0.48
1:B:684:SER:HB3	1:C:1008:ARG:HD2	1.96	0.48
1:B:723:TYR:OH	1:B:756:VAL:HG11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:916:MET:HE1	1:C:960:LEU:HA	1.95	0.48
1:B:681:ARG:NH1	1:B:975:GLY:O	2.44	0.47
1:D:687:SER:O	1:D:691:GLU:HG3	2.14	0.47
1:A:778:VAL:O	1:A:782:VAL:HG23	2.14	0.47
1:A:902:MET:HE3	1:A:906:GLU:CG	2.43	0.47
1:C:775:VAL:HG22	1:C:817:SER:HA	1.95	0.47
1:A:723:TYR:OH	1:A:756:VAL:HG11	2.15	0.47
1:A:775:VAL:HG22	1:A:817:SER:HA	1.96	0.47
1:A:916:MET:HE2	1:A:960:LEU:HD23	1.95	0.47
1:C:936:VAL:CG1	1:C:937:GLU:N	2.78	0.47
1:D:902:MET:HE1	1:D:1013:ALA:CA	2.44	0.47
1:A:860:MET:HE3	1:A:890:VAL:HG21	1.96	0.47
1:D:916:MET:HE3	1:D:959:GLN:HB3	1.96	0.46
1:C:687:SER:O	1:C:691:GLU:HG3	2.15	0.46
1:D:916:MET:HE1	1:D:960:LEU:HA	1.96	0.46
1:C:686:TRP:CZ2	1:C:695:ARG:HD2	2.51	0.46
1:A:715:HIS:CE1	1:A:816:ASN:H	2.19	0.46
1:A:660:THR:HG21	5:A:2001:HOH:O	2.16	0.45
1:B:688:ARG:O	1:B:692:THR:HG22	2.16	0.45
1:C:716:SER:O	1:C:720:THR:HG23	2.17	0.45
1:C:936:VAL:HG12	1:C:937:GLU:N	2.31	0.45
1:B:892:MET:HE3	1:B:914:VAL:HB	1.99	0.44
1:D:927:VAL:HG13	1:D:968:ILE:HA	2.00	0.44
1:C:925:ASP:O	1:C:967:ARG:NH1	2.50	0.44
1:D:925:ASP:O	1:D:967:ARG:NH1	2.51	0.44
1:A:686:TRP:CZ2	1:A:695:ARG:HD2	2.53	0.44
1:A:925:ASP:O	1:A:967:ARG:NH1	2.50	0.44
1:A:665:HIS:CD2	1:A:767:SER:OG	2.71	0.44
1:D:722:LEU:O	1:D:730:ARG:NH1	2.51	0.44
1:C:860:MET:HE1	1:C:915:VAL:HA	1.99	0.43
1:B:925:ASP:O	1:B:967:ARG:NH1	2.51	0.43
1:D:686:TRP:CZ2	1:D:695:ARG:HD2	2.53	0.43
1:D:903:GLY:HA2	1:D:948:LEU:HD12	2.00	0.43
1:A:658:TYR:CE1	1:A:682:ILE:HG22	2.53	0.43
1:A:880:VAL:HG13	1:A:887:GLY:H	1.83	0.43
1:B:656:LEU:HD12	1:B:698:CYS:HB2	2.00	0.43
1:B:955:TYR:CZ	1:B:1000:LEU:HD13	2.53	0.43
1:D:841:VAL:HG12	1:D:934:ASP:CG	2.43	0.43
1:B:892:MET:CE	1:B:914:VAL:CB	2.96	0.43
1:C:704:ARG:O	1:C:776:GLY:HA3	2.19	0.43
1:D:692:THR:HG21	1:D:694:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:TYR:HE1	1:A:682:ILE:CG2	2.31	0.43
1:B:892:MET:CE	1:B:914:VAL:HG21	2.37	0.42
1:C:711:LEU:HD11	1:C:772:ARG:HG2	2.01	0.42
1:C:902:MET:HE1	1:C:1013:ALA:CA	2.49	0.42
1:D:704:ARG:O	1:D:776:GLY:HA3	2.19	0.42
1:D:841:VAL:HA	5:D:2012:HOH:O	2.20	0.42
1:B:659:ASP:CG	1:B:773:LEU:HD21	2.44	0.42
1:C:722:LEU:O	1:C:730:ARG:NH1	2.53	0.42
1:A:704:ARG:O	1:A:776:GLY:HA3	2.19	0.42
1:C:843:HIS:CD2	1:C:874:SER:OG	2.67	0.42
1:C:860:MET:HE2	1:C:860:MET:HB3	1.92	0.42
1:B:902:MET:CE	1:B:1013:ALA:HB2	2.34	0.42
1:B:762:TRP:CZ3	1:B:767:SER:HB3	2.55	0.42
1:C:902:MET:CE	1:C:1013:ALA:HB2	2.45	0.42
1:C:783:PHE:CE1	1:C:825:LEU:HD23	2.55	0.42
1:A:656:LEU:HD23	1:A:794:PHE:HB3	2.00	0.41
1:A:902:MET:HE3	1:A:906:GLU:HB3	2.02	0.41
1:C:860:MET:CE	1:C:890:VAL:HG11	2.38	0.41
1:D:728:ALA:HB3	5:D:2006:HOH:O	2.20	0.41
1:C:782:VAL:CG1	1:C:825:LEU:HD11	2.50	0.41
1:D:1029:ARG:O	1:D:1032:GLN:HG3	2.19	0.41
1:B:704:ARG:O	1:B:776:GLY:HA3	2.21	0.41
1:A:762:TRP:CZ3	1:A:767:SER:HB3	2.56	0.41
1:A:866:ASP:O	1:A:867:ASP:CB	2.65	0.41
1:B:902:MET:HE3	1:B:906:GLU:HB3	2.02	0.41
1:C:728:ALA:HB3	5:C:2010:HOH:O	2.19	0.41
1:C:816:ASN:HD22	1:C:816:ASN:C	2.27	0.41
1:A:866:ASP:O	1:A:867:ASP:HB3	2.21	0.41
1:D:762:TRP:CZ3	1:D:767:SER:HB3	2.57	0.40
1:B:892:MET:CE	1:B:914:VAL:CG1	2.99	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	378/395 (96%)	363 (96%)	15 (4%)	0	100	100
1	B	378/395 (96%)	361 (96%)	17 (4%)	0	100	100
1	C	378/395 (96%)	364 (96%)	13 (3%)	1 (0%)	36	59
1	D	381/395 (96%)	365 (96%)	15 (4%)	1 (0%)	36	59
All	All	1515/1580 (96%)	1453 (96%)	60 (4%)	2 (0%)	48	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	671	SER
1	D	671	SER

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	297/321 (92%)	287 (97%)	10 (3%)	32	60
1	B	290/321 (90%)	283 (98%)	7 (2%)	43	70
1	C	292/321 (91%)	281 (96%)	11 (4%)	29	56
1	D	291/321 (91%)	281 (97%)	10 (3%)	32	60
All	All	1170/1284 (91%)	1132 (97%)	38 (3%)	34	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	671	SER
1	A	677	GLU
1	A	682	ILE
1	A	735	SER
1	A	745	VAL
1	A	880	VAL

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Mol	Chain	Res	Type
1	A	895	THR
1	A	934	ASP
1	A	941	THR
1	A	947	ASN
1	B	666	GLN
1	B	671	SER
1	B	677	GLU
1	B	722	LEU
1	B	911	PHE
1	B	934	ASP
1	B	1004	VAL
1	C	677	GLU
1	C	732	LYS
1	C	735	SER
1	C	745	VAL
1	C	827	GLN
1	C	880	VAL
1	C	895	THR
1	C	911	PHE
1	C	1002	GLU
1	C	1006	GLN
1	C	1022	GLU
1	D	666	GLN
1	D	671	SER
1	D	677	GLU
1	D	745	VAL
1	D	764	GLU
1	D	895	THR
1	D	911	PHE
1	D	927	VAL
1	D	934	ASP
1	D	1033	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	665	HIS
1	A	678	HIS
1	A	712	GLN
1	A	715	HIS
1	A	947	ASN
1	A	995	ASN

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Mol	Chain	Res	Type
1	A	1012	ASN
1	A	1024	HIS
1	B	666	GLN
1	B	712	GLN
1	B	729	ASN
1	B	843	HIS
1	B	995	ASN
1	B	1024	HIS
1	C	666	GLN
1	C	678	HIS
1	C	729	ASN
1	C	731	GLN
1	C	816	ASN
1	C	827	GLN
1	C	843	HIS
1	C	959	GLN
1	C	995	ASN
1	D	665	HIS
1	D	666	GLN
1	D	690	GLN
1	D	729	ASN
1	D	731	GLN
1	D	766	HIS
1	D	995	ASN
1	D	1024	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	KEE	B	2032	3	26,27,27	1.32	3 (11%)	33,38,38	1.73	7 (21%)
2	KEE	C	2033	3	26,27,27	1.26	4 (15%)	33,38,38	1.77	7 (21%)
2	KEE	A	2033	3	26,27,27	1.14	2 (7%)	33,38,38	2.14	10 (30%)
2	KEE	D	2036	3	26,27,27	1.09	2 (7%)	33,38,38	1.86	5 (15%)

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	KEE	B	2032	3	-	2/18/27/27	0/4/4/4
2	KEE	C	2033	3	-	1/18/27/27	0/4/4/4
2	KEE	A	2033	3	-	6/18/27/27	0/4/4/4
2	KEE	D	2036	3	-	4/18/27/27	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2032	KEE	C21-C17	3.53	1.40	1.34
2	C	2033	KEE	C21-C17	3.33	1.39	1.34
2	A	2033	KEE	C21-C17	3.19	1.39	1.34
2	D	2036	KEE	C21-C17	3.02	1.39	1.34
2	C	2033	KEE	C19-N20	2.76	1.36	1.28
2	B	2032	KEE	C19-N20	2.73	1.36	1.28
2	D	2036	KEE	C19-N20	2.60	1.36	1.28
2	A	2033	KEE	C19-N20	2.53	1.36	1.28
2	C	2033	KEE	C2-C3	2.07	1.55	1.52
2	B	2032	KEE	O18-C19	2.05	1.39	1.35
2	C	2033	KEE	O18-C19	2.04	1.39	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2033	KEE	C8-C17-C21	-7.39	126.32	135.21
2	C	2033	KEE	C8-C17-C21	-6.74	127.10	135.21
2	B	2032	KEE	C8-C17-C21	-6.67	127.18	135.21
2	D	2036	KEE	C8-C17-C21	-6.57	127.30	135.21
2	A	2033	KEE	C5-C3-C2	-4.80	112.38	121.60
2	D	2036	KEE	C5-C3-C2	-4.44	113.08	121.60
2	D	2036	KEE	C11-C4-C3	-3.39	113.45	121.73
2	A	2033	KEE	C11-C4-C3	-3.29	113.69	121.73
2	B	2032	KEE	C11-C4-C3	-3.19	113.94	121.73
2	A	2033	KEE	O18-C19-N20	-2.97	108.00	114.64
2	C	2033	KEE	C5-C3-C2	-2.93	115.99	121.60
2	C	2033	KEE	O18-C19-N20	-2.87	108.23	114.64
2	B	2032	KEE	O18-C19-N20	-2.86	108.26	114.64
2	B	2032	KEE	O22-C1-C2	2.80	128.29	122.36
2	A	2033	KEE	C7-C8-C17	-2.62	116.61	120.77
2	C	2033	KEE	O22-C1-C2	2.57	127.81	122.36
2	D	2036	KEE	O18-C19-N20	-2.50	109.06	114.64
2	A	2033	KEE	O18-C17-C8	2.48	126.41	118.34
2	B	2032	KEE	O18-C17-C8	2.43	126.26	118.34
2	A	2033	KEE	C2-C1-N23	-2.41	109.62	114.85
2	A	2033	KEE	O22-C1-C2	2.36	127.37	122.36
2	B	2032	KEE	C5-C3-C2	-2.29	117.20	121.60
2	C	2033	KEE	C21-N20-C19	2.26	109.14	104.05
2	B	2032	KEE	C4-C2-C1	2.26	125.23	119.45
2	A	2033	KEE	C21-N20-C19	2.20	108.99	104.05
2	C	2033	KEE	C2-C1-N23	-2.12	110.24	114.85
2	A	2033	KEE	C3-C2-C1	2.08	124.77	119.45
2	C	2033	KEE	O18-C17-C8	2.01	124.88	118.34
2	D	2036	KEE	O22-C1-C2	2.01	126.61	122.36

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2033	KEE	O18-C17-C8-C7
2	A	2033	KEE	O18-C17-C8-C9
2	A	2033	KEE	C21-C17-C8-C7
2	A	2033	KEE	C21-C17-C8-C9
2	A	2033	KEE	O22-C1-C2-C4
2	A	2033	KEE	N23-C1-C2-C4
2	B	2032	KEE	O22-C1-C2-C4

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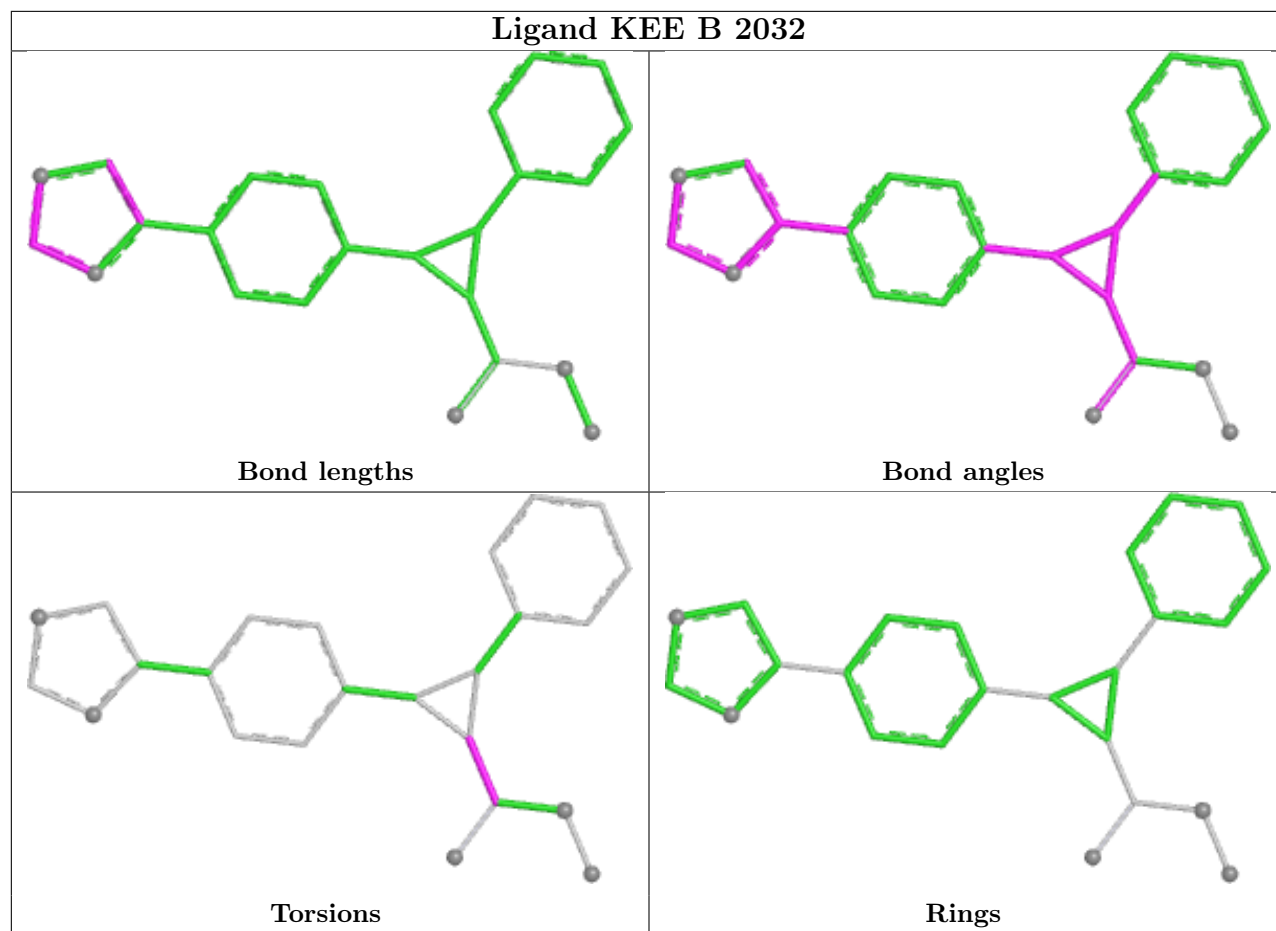
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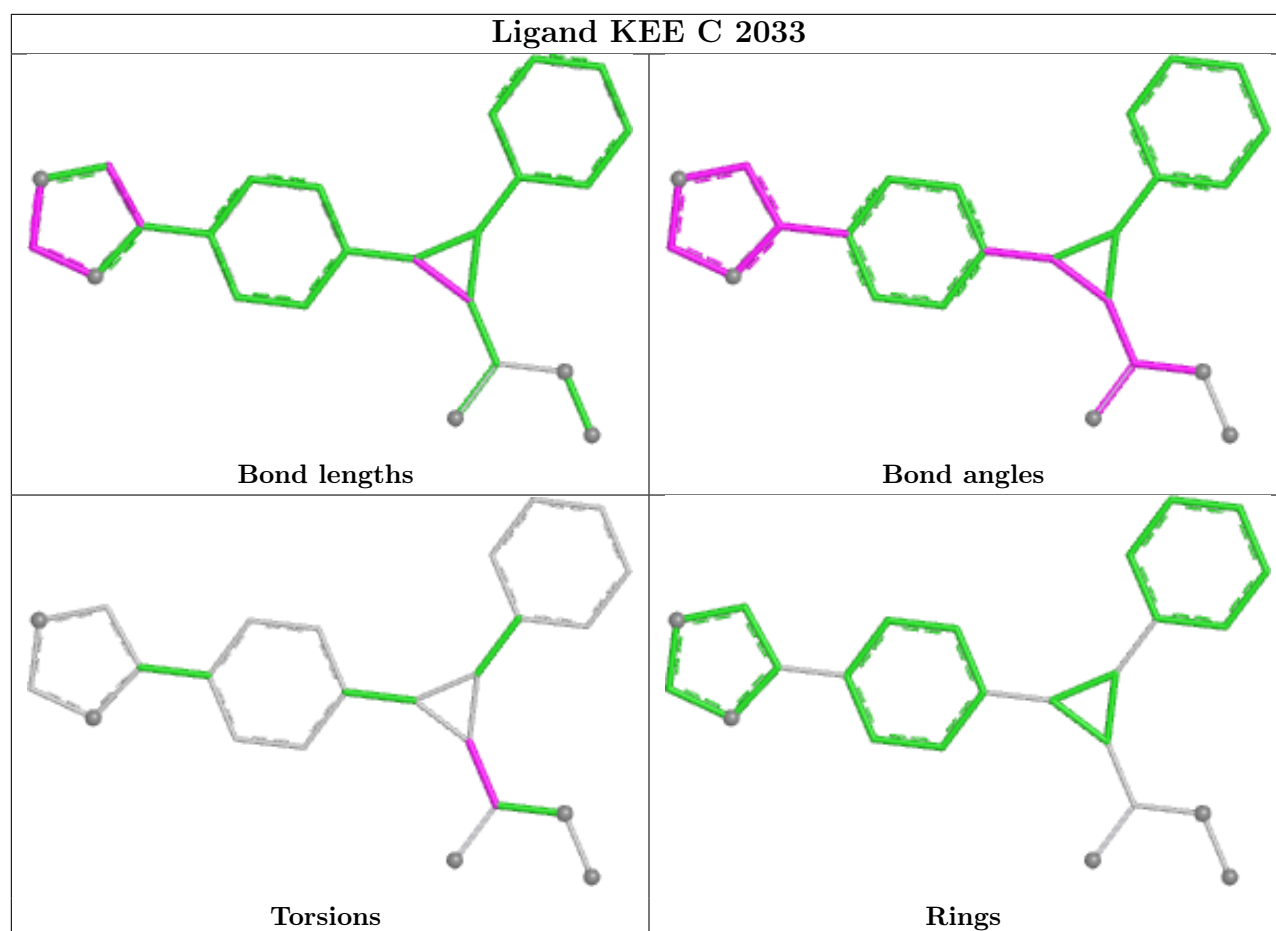
Mol	Chain	Res	Type	Atoms
2	D	2036	KEE	O22-C1-C2-C4
2	D	2036	KEE	N23-C1-C2-C4
2	D	2036	KEE	C4-C3-C5-C6
2	B	2032	KEE	N23-C1-C2-C4
2	C	2033	KEE	N23-C1-C2-C4
2	D	2036	KEE	C4-C3-C5-C10

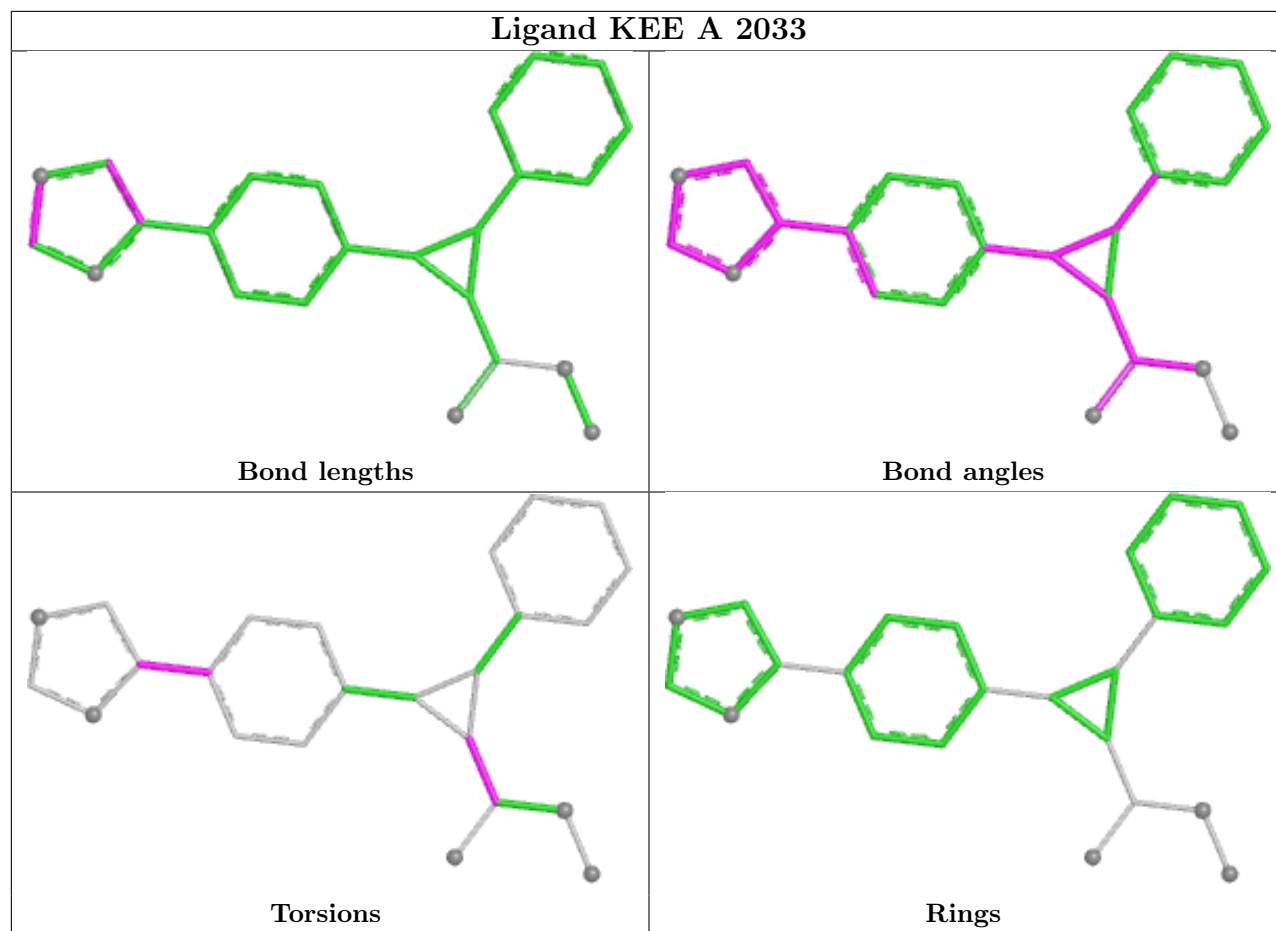
There are no ring outliers.

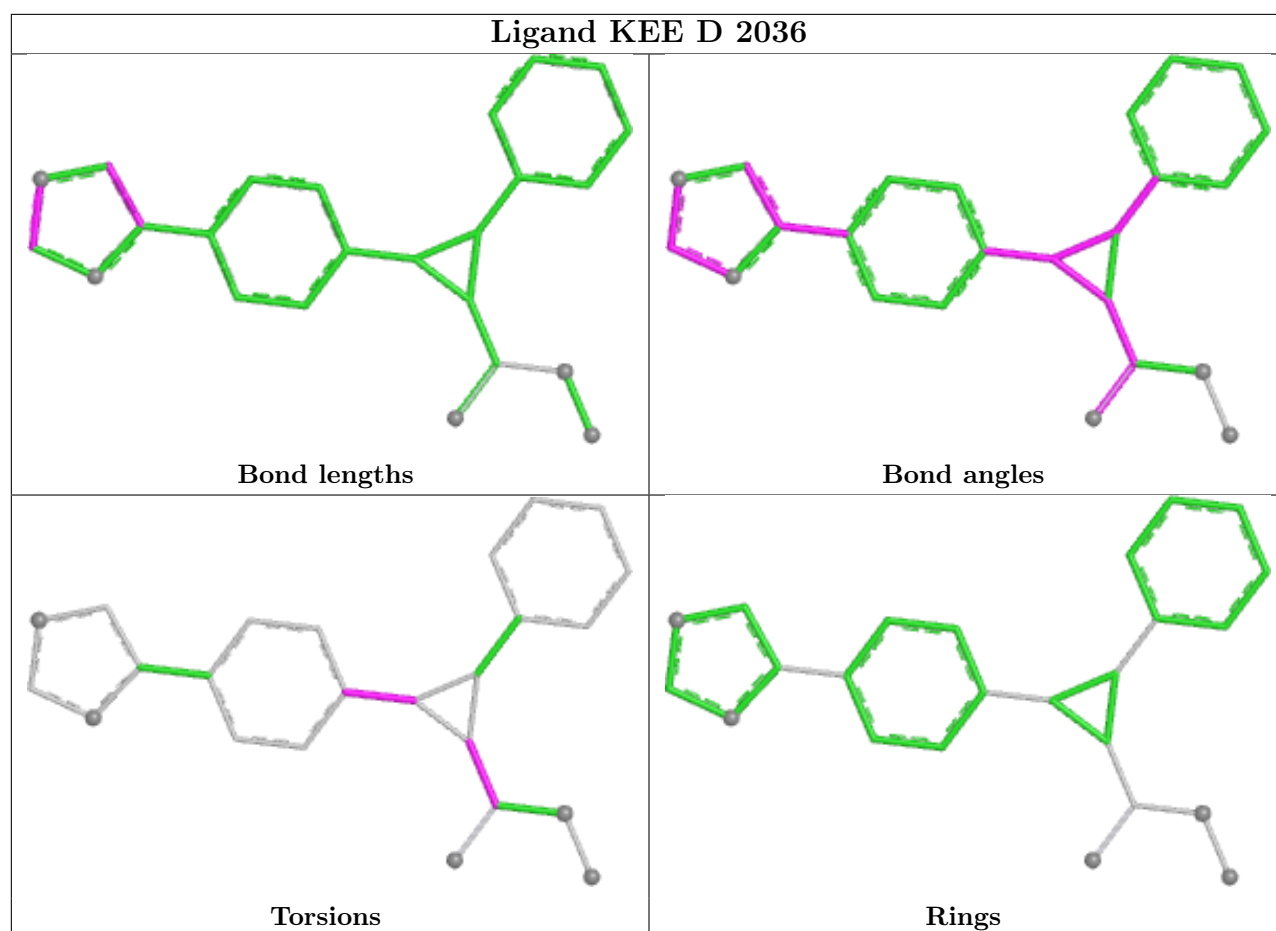
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	380/395 (96%)	-0.23	1 (0%) 90 89	15, 29, 45, 57	0
1	B	380/395 (96%)	-0.26	1 (0%) 90 89	16, 28, 45, 57	0
1	C	380/395 (96%)	-0.22	2 (0%) 87 86	18, 29, 54, 79	0
1	D	383/395 (96%)	-0.17	1 (0%) 90 89	20, 31, 55, 78	0
All	All	1523/1580 (96%)	-0.22	5 (0%) 90 89	15, 29, 50, 79	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	673	SER	4.1
1	B	941	THR	3.3
1	A	867	ASP	2.9
1	D	941	THR	2.5
1	C	671	SER	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

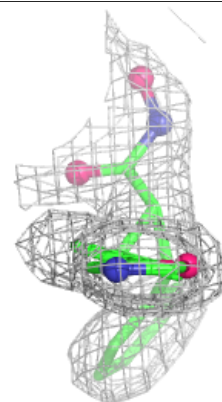
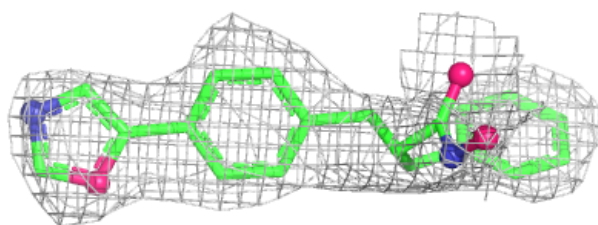
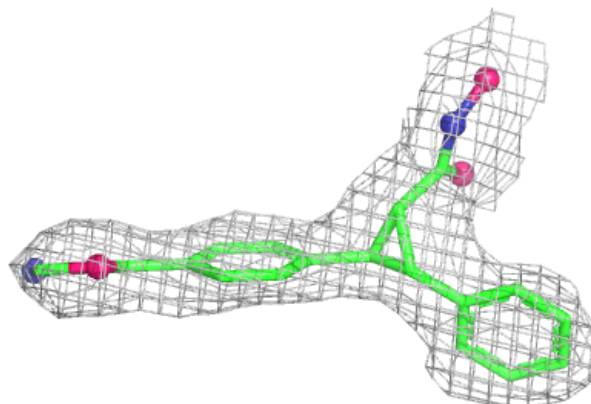
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	B	2035	1/1	0.68	0.11	28,28,28,28	0
4	NA	D	2040	1/1	0.82	0.09	24,24,24,24	0
4	NA	A	2036	1/1	0.83	0.08	28,28,28,28	0
4	NA	C	2037	1/1	0.86	0.08	22,22,22,22	0
4	NA	C	2036	1/1	0.87	0.09	25,25,25,25	0
4	NA	B	2036	1/1	0.88	0.09	23,23,23,23	0
4	NA	D	2039	1/1	0.90	0.10	23,23,23,23	0
4	NA	A	2037	1/1	0.92	0.07	20,20,20,20	0
2	KEE	D	2036	24/24	0.93	0.09	28,33,41,43	0
2	KEE	A	2033	24/24	0.95	0.08	24,28,37,38	0
2	KEE	B	2032	24/24	0.95	0.08	23,26,35,36	0
2	KEE	C	2033	24/24	0.95	0.09	26,29,37,38	0
3	ZN	C	2035	1/1	0.98	0.03	46,46,46,46	0
3	ZN	B	2033	1/1	0.99	0.02	23,23,23,23	0
3	ZN	B	2034	1/1	0.99	0.02	28,28,28,28	0
3	ZN	A	2035	1/1	0.99	0.02	25,25,25,25	0
3	ZN	D	2038	1/1	0.99	0.02	45,45,45,45	0
3	ZN	C	2034	1/1	1.00	0.01	25,25,25,25	0
3	ZN	A	2034	1/1	1.00	0.01	19,19,19,19	0
3	ZN	D	2037	1/1	1.00	0.01	25,25,25,25	0

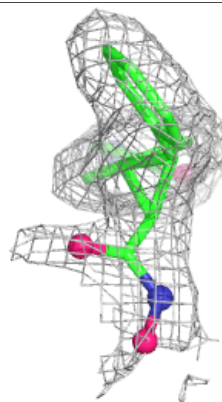
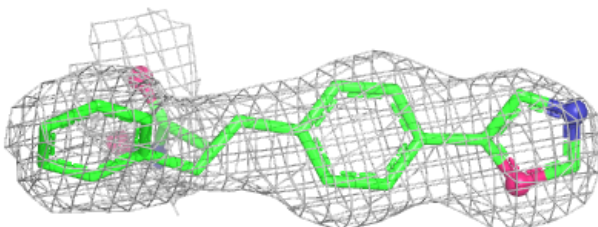
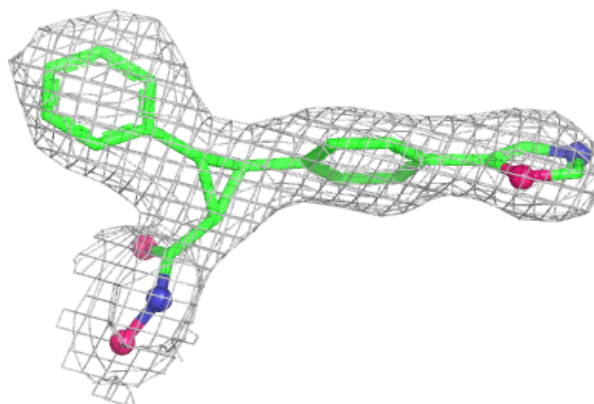
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KEE D 2036:

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

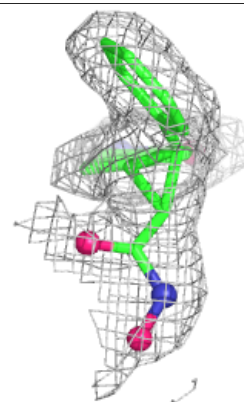
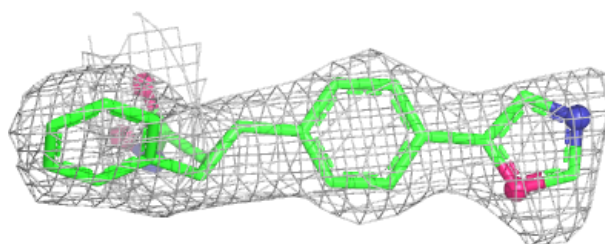
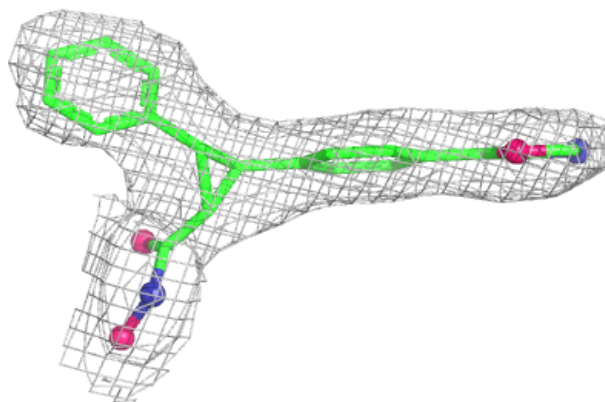
**Electron density around KEE A 2033:**

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

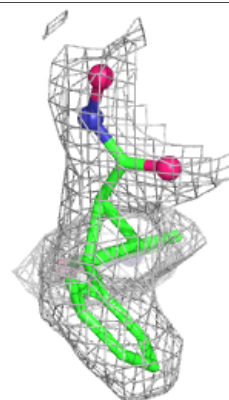
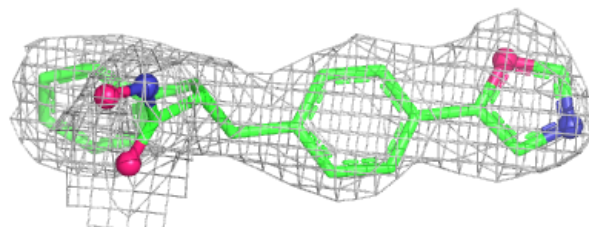
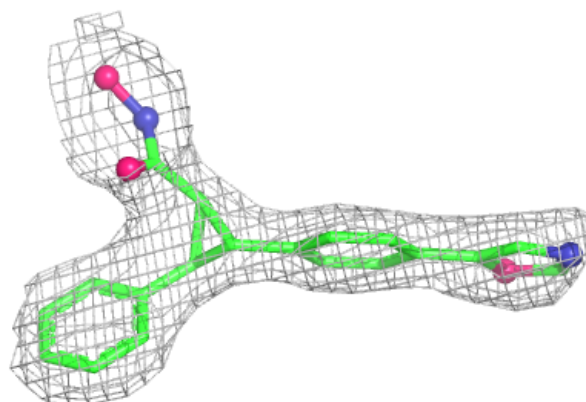


Electron density around KEE B 2032:

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

**Electron density around KEE C 2033:**

$2mF_o-DF_c$ (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.