Full wwPDB X-ray Structure Validation Report (i)

May 5, 2022 – 10:53 am BST

PDB ID	:	7PWY
Title	:	Structure of human dimeric ACMSD in complex with the inhibitor TES-1025
Authors	:	Cianci, M.; Giacche, N.; Carotti, A.; Liscio, P.; Amici, A.; Cialabrini, L.; De Franco, F.; Pellicciari, R.; Raffaelli, N.
Deposited on	:	2021-10-07
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.50 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.9%
RSRZ outliers		6.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
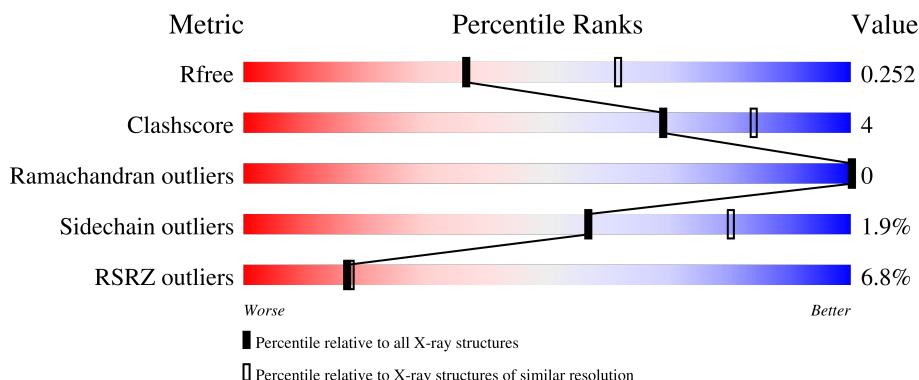
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	4% / 89% / 10% ·
1	B	336	4% / 89% / 10% ··
1	C	336	10% / 81% / 8% · 10%
1	D	336	10% / 82% / 12% · 5%
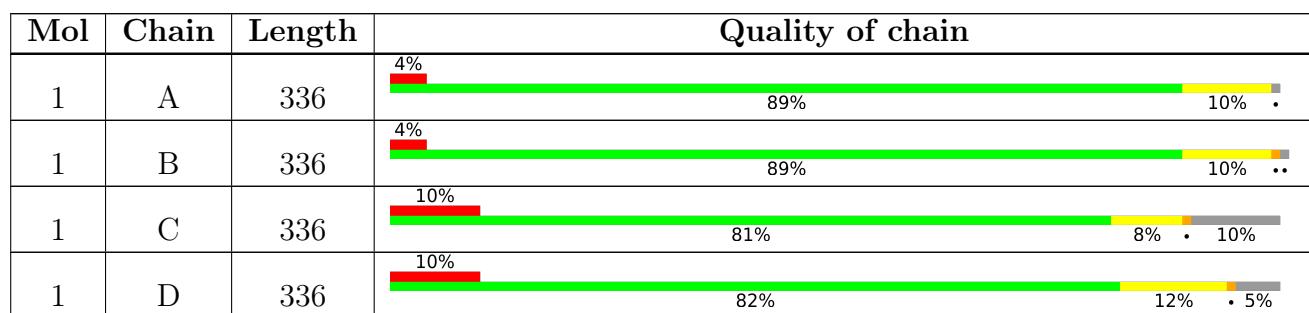
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10647 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 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2668	1726	449	473	20			
1	B	334	Total	C	N	O	S	0	3	0
			2674	1731	449	474	20			
1	C	301	Total	C	N	O	S	0	1	0
			2399	1566	394	425	14			
1	D	320	Total	C	N	O	S	0	2	0
			2555	1659	429	450	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-[3-[(5-cyano-6-oxidanylidene-4-thiophen-2-yl-1H-pyrimidin-2-yl)sulfanyl methyl]phenyl]ethanoic acid (three-letter code: 8EK) (formula: $C_{18}H_{13}N_3O_3S_2$) (labeled as "Ligand of Interest" by depositor).
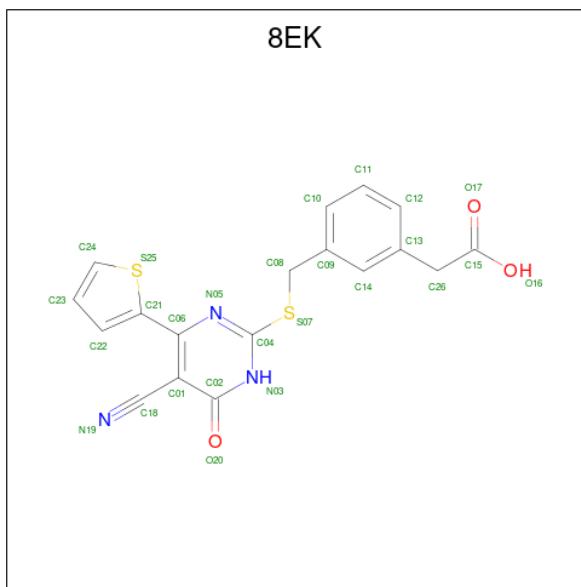
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	18	3	3	2		
3	B	1	Total	C	N	O	S	0	0
			26	18	3	3	2		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	146	Total	O	0	0
			146	146		
5	B	93	Total	O	0	0
			93	93		
5	C	25	Total	O	0	0
			25	25		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	25	Total　O 25　　25		0	0

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: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase
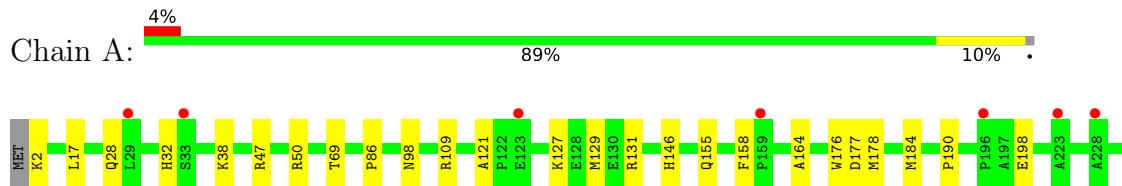
Chain A:

- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

Chain B:

- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

Chain C:

- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

Chain D:
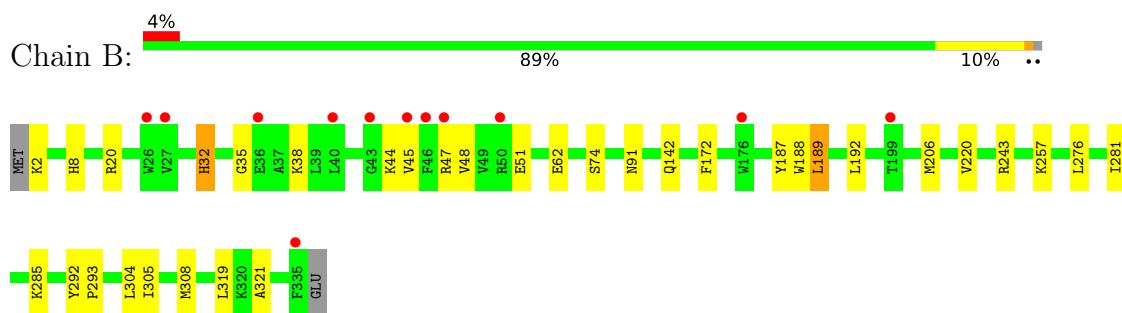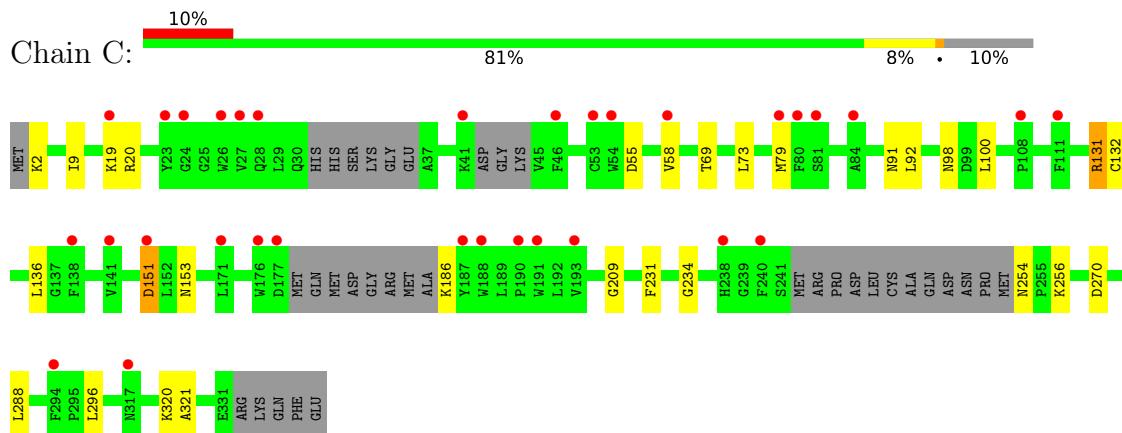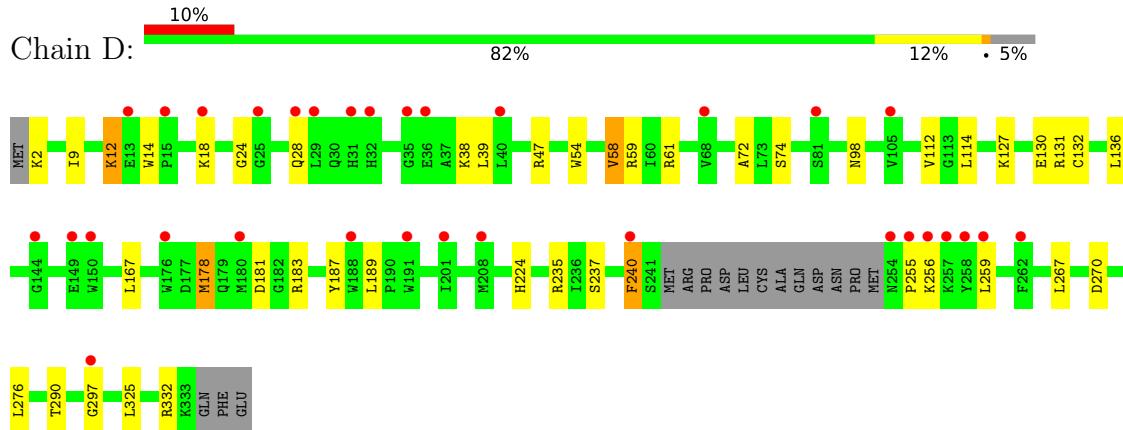
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	153.41Å 92.58Å 103.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.33 – 2.50 45.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.33-2.50) 99.3 (45.33-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.210 , 0.252 0.210 , 0.252	Depositor DCC
R_{free} test set	2565 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10647	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8EK, ZN, K

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	0.25	0/2746	0.48	0/3715
1	B	0.25	0/2755	0.47	0/3726
1	C	0.24	0/2465	0.45	0/3337
1	D	0.25	0/2629	0.46	0/3553
All	All	0.25	0/10595	0.47	0/14331

There are no bond length outliers.

There are no bond angle outliers.

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	2668	0	2676	19	0
1	B	2674	0	2687	20	0
1	C	2399	0	2410	15	0
1	D	2555	0	2580	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	146	0	0	1	0
5	B	93	0	0	1	0
5	C	25	0	0	0	0
5	D	25	0	0	2	0
All	All	10647	0	10353	76	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 4.

All (76) 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:130:GLU:HG2	1:D:167:LEU:HD11	1.68	0.74
1:A:50:ARG:NH2	5:A:501:HOH:O	2.20	0.74
1:A:17:LEU:H	1:A:28:GLN:HE22	1.37	0.72
1:A:98:ASN:OD1	1:A:131:ARG:NH2	2.24	0.70
1:A:2:LYS:HB3	1:A:321:ALA:HB2	1.76	0.67
1:B:20:ARG:NH1	1:B:91:ASN:OD1	2.27	0.67
1:C:2:LYS:HB3	1:C:321:ALA:HB2	1.79	0.64
1:B:47:ARG:HG2	3:B:402:8EK:S07	2.40	0.61
1:C:55:ASP:HB3	1:C:58:VAL:HG22	1.83	0.61
1:A:129:MET:HE3	1:A:164:ALA:HA	1.83	0.61
1:B:44:LYS:NZ	5:B:506:HOH:O	2.34	0.60
1:A:47:ARG:HD2	3:A:402:8EK:S07	2.42	0.60
1:D:235:ARG:NH1	5:D:501:HOH:O	2.33	0.59
1:C:2:LYS:HB2	1:C:320:LYS:HB3	1.84	0.59
1:B:187:TYR:HB2	1:B:189:LEU:HD22	1.86	0.57
1:A:17:LEU:H	1:A:28:GLN:NE2	2.04	0.55
1:C:132:CYS:HA	1:C:136:LEU:HD23	1.90	0.54
1:A:243:ARG:HH21	1:A:246:LEU:HD11	1.73	0.53
1:D:2[A]:LYS:NZ	5:D:502:HOH:O	2.42	0.53
1:D:224:HIS:HD2	1:D:267:LEU:HD23	1.74	0.52
1:B:47:ARG:HE	1:B:48:VAL:H	1.56	0.52
1:D:240:PHE:HD2	1:D:255:PRO:HD3	1.75	0.52
1:D:14:TRP:HE1	1:D:28:GLN:HA	1.76	0.51
1:C:153:ASN:HB2	1:C:209:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:SER:HB3	1:D:114:LEU:HB2	1.93	0.50
1:D:132:CYS:HA	1:D:136:LEU:HD23	1.93	0.50
1:A:276:LEU:HD22	1:B:276:LEU:HD22	1.94	0.49
1:A:32:HIS:CD2	1:A:38:LYS:HG3	2.48	0.49
1:D:98:ASN:OD1	1:D:131:ARG:NH2	2.45	0.49
1:D:224:HIS:CD2	1:D:267:LEU:HD23	2.47	0.49
1:C:288:LEU:HD12	1:C:320:LYS:HA	1.95	0.49
1:C:20:ARG:NH1	1:C:91:ASN:OD1	2.44	0.48
1:C:254:ASN:OD1	1:C:256:LYS:HG2	2.14	0.48
1:D:12:LYS:HG3	1:D:54:TRP:HD1	1.79	0.48
1:D:178:MET:SD	1:D:178:MET:N	2.74	0.48
1:B:35:GLY:HA2	1:B:51:GLU:HG3	1.94	0.48
1:B:305:ILE:HD13	1:B:319:LEU:HB3	1.95	0.48
1:B:142:GLN:HG3	1:B:172:PHE:HD2	1.80	0.46
1:D:39:LEU:HD12	1:D:47:ARG:HB3	1.96	0.46
1:A:2:LYS:HG2	1:A:69:THR:OG1	2.15	0.46
1:A:86:PRO:HB3	1:A:121:ALA:HB2	1.98	0.46
1:B:2:LYS:HB2	1:B:321:ALA:HB2	1.98	0.46
1:B:62:GLU:OE1	1:B:292:TYR:OH	2.30	0.45
1:D:256:LYS:HA	1:D:259:LEU:HD23	1.96	0.45
1:D:325:LEU:HD13	1:D:332:ARG:HG2	1.99	0.45
1:D:18:LYS:HE3	1:D:24:GLY:HA3	1.99	0.45
1:A:239:GLY:HA3	1:B:192:LEU:HD21	1.98	0.45
1:A:184:MET:O	1:A:190:PRO:HD3	2.17	0.44
1:D:12:LYS:HG3	1:D:54:TRP:CD1	2.52	0.44
1:C:151:ASP:OD2	1:D:183:ARG:NH2	2.33	0.43
1:B:206:MET:HE1	1:B:220:VAL:HG21	2.00	0.43
1:D:127:LYS:HE3	1:D:127:LYS:HB2	1.69	0.43
1:D:290:THR:O	1:D:297:GLY:HA3	2.19	0.43
1:C:2:LYS:O	1:C:69:THR:N	2.45	0.43
1:A:47:ARG:HH11	1:B:243:ARG:HH11	1.67	0.42
1:B:304:LEU:O	1:B:308:MET:HG2	2.18	0.42
1:C:79:MET:HE3	1:C:92:LEU:HD21	2.01	0.42
1:C:231:PHE:CD1	1:D:276:LEU:HD23	2.54	0.42
1:D:181:ASP:OD1	1:D:181:ASP:N	2.43	0.42
1:A:331:GLU:O	1:A:333:LYS:HG2	2.20	0.42
1:B:38:LYS:HD2	1:B:45:VAL:HG21	2.02	0.42
1:B:8:HIS:HA	1:B:74:SER:O	2.20	0.42
1:D:9:ILE:HD12	1:D:59:ARG:NH1	2.35	0.42
1:A:146:HIS:HD2	1:A:198:GLU:OE1	2.03	0.42
1:A:155:GLN:HA	1:A:158:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:TYR:HB2	1:D:189:LEU:HD13	2.02	0.41
1:D:58:VAL:O	1:D:61:ARG:HG2	2.21	0.41
1:D:72:ALA:HA	1:D:112:VAL:HG23	2.00	0.41
1:A:176:TRP:CG	1:A:177:ASP:N	2.88	0.41
1:B:281:ILE:HG22	1:B:285:LYS:HB2	2.03	0.41
1:C:9:ILE:HB	1:C:73:LEU:HD12	2.03	0.41
1:C:234:GLY:HA3	1:D:270:ASP:HB2	2.03	0.41
1:D:237:SER:OG	1:D:256:LYS:HG2	2.21	0.41
1:B:32:HIS:H	1:B:32:HIS:CD2	2.39	0.40
1:C:98:ASN:HD21	1:C:131:ARG:NH2	2.19	0.40
1:B:292:TYR:HA	1:B:293:PRO:HA	1.89	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	334/336 (99%)	324 (97%)	10 (3%)	0	100	100
1	B	335/336 (100%)	325 (97%)	10 (3%)	0	100	100
1	C	292/336 (87%)	281 (96%)	11 (4%)	0	100	100
1	D	317/336 (94%)	304 (96%)	13 (4%)	0	100	100
All	All	1278/1344 (95%)	1234 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	289/289 (100%)	284 (98%)	5 (2%)	60	82
1	B	290/289 (100%)	286 (99%)	4 (1%)	67	86
1	C	260/289 (90%)	253 (97%)	7 (3%)	44	71
1	D	276/289 (96%)	271 (98%)	5 (2%)	59	81
All	All	1115/1156 (96%)	1094 (98%)	21 (2%)	57	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	127	LYS
1	A	178	MET
1	A	291	ASP
1	A	299	LEU
1	B	32	HIS
1	B	188	TRP
1	B	189	LEU
1	B	257	LYS
1	C	19	LYS
1	C	100	LEU
1	C	131	ARG
1	C	151	ASP
1	C	186	LYS
1	C	270	ASP
1	C	296	LEU
1	D	12	LYS
1	D	38	LYS
1	D	58	VAL
1	D	178	MET
1	D	240	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	32	HIS
1	A	224	HIS
1	B	32	HIS

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Mol	Chain	Res	Type
1	D	32	HIS
1	D	94	GLN
1	D	224	HIS
1	D	269	HIS

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 12 ligands modelled in this entry, 10 are monoatomic - 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	#$|Z| > 2$
3	8EK	A	402	2	25,28,28	4.73	16 (64%)	24,38,38	3.05	6 (25%)
3	8EK	B	402	2	25,28,28	4.63	16 (64%)	24,38,38	3.20	7 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8EK	A	402	2	-	7/8/15/15	0/3/3/3
3	8EK	B	402	2	-	6/8/15/15	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	8EK	C04-S07	11.82	1.97	1.75
3	B	402	8EK	C04-S07	11.81	1.97	1.75
3	B	402	8EK	C06-N05	9.56	1.49	1.34
3	A	402	8EK	C02-N03	9.39	1.49	1.33
3	A	402	8EK	C06-N05	9.17	1.49	1.34
3	B	402	8EK	C02-N03	8.93	1.48	1.33
3	B	402	8EK	C06-C21	6.30	1.63	1.49
3	A	402	8EK	C06-C21	6.23	1.62	1.49
3	A	402	8EK	C01-C18	5.54	1.50	1.44
3	A	402	8EK	C04-N03	5.51	1.42	1.34
3	B	402	8EK	C04-N03	5.19	1.41	1.34
3	B	402	8EK	C01-C18	5.15	1.50	1.44
3	A	402	8EK	C08-S07	4.99	1.93	1.82
3	A	402	8EK	C01-C02	4.87	1.56	1.43
3	B	402	8EK	C08-S07	4.68	1.92	1.82
3	B	402	8EK	C01-C02	4.62	1.55	1.43
3	A	402	8EK	C14-C09	4.50	1.47	1.39
3	B	402	8EK	C21-S25	4.07	1.76	1.72
3	B	402	8EK	C14-C09	3.81	1.45	1.39
3	A	402	8EK	C21-S25	3.78	1.76	1.72
3	B	402	8EK	C23-C22	3.51	1.51	1.39
3	A	402	8EK	C23-C22	3.46	1.50	1.39
3	A	402	8EK	C08-C09	3.34	1.58	1.51
3	A	402	8EK	C14-C13	3.17	1.44	1.39
3	A	402	8EK	C12-C13	3.13	1.45	1.38
3	B	402	8EK	C08-C09	3.10	1.58	1.51
3	B	402	8EK	C12-C13	2.84	1.45	1.38
3	B	402	8EK	C14-C13	2.70	1.43	1.39
3	A	402	8EK	C11-C10	2.55	1.44	1.38
3	B	402	8EK	C11-C10	2.48	1.44	1.38
3	A	402	8EK	C26-C13	2.10	1.58	1.52
3	B	402	8EK	C26-C13	2.05	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	8EK	C08-S07-C04	10.51	113.98	102.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	8EK	C08-S07-C04	10.20	113.63	102.42
3	A	402	8EK	C01-C02-N03	-7.66	117.30	124.09
3	B	402	8EK	C01-C02-N03	-7.52	117.42	124.09
3	B	402	8EK	C23-C24-S25	-5.02	108.91	112.98
3	A	402	8EK	C23-C24-S25	-4.33	109.47	112.98
3	B	402	8EK	C04-N03-C02	3.69	120.02	115.79
3	A	402	8EK	C04-N03-C02	3.53	119.84	115.79
3	A	402	8EK	N05-C04-N03	-2.54	122.30	126.95
3	B	402	8EK	C09-C14-C13	2.35	124.12	121.23
3	B	402	8EK	N05-C04-N03	-2.35	122.65	126.95
3	B	402	8EK	C21-C06-N05	2.30	119.38	115.10
3	A	402	8EK	C09-C14-C13	2.03	123.73	121.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	8EK	N03-C04-S07-C08
3	A	402	8EK	N05-C04-S07-C08
3	B	402	8EK	N03-C04-S07-C08
3	B	402	8EK	N05-C04-S07-C08
3	B	402	8EK	S07-C08-C09-C10
3	A	402	8EK	S07-C08-C09-C10
3	A	402	8EK	S07-C08-C09-C14
3	B	402	8EK	S07-C08-C09-C14
3	A	402	8EK	C09-C08-S07-C04
3	B	402	8EK	C12-C13-C26-C15
3	B	402	8EK	C14-C13-C26-C15
3	A	402	8EK	C12-C13-C26-C15
3	A	402	8EK	C14-C13-C26-C15

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	8EK	1	0
3	B	402	8EK	1	0

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

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

Ligand 8EK A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 8EK B 402

Bond lengths

Bond angles

Torsions

Rings
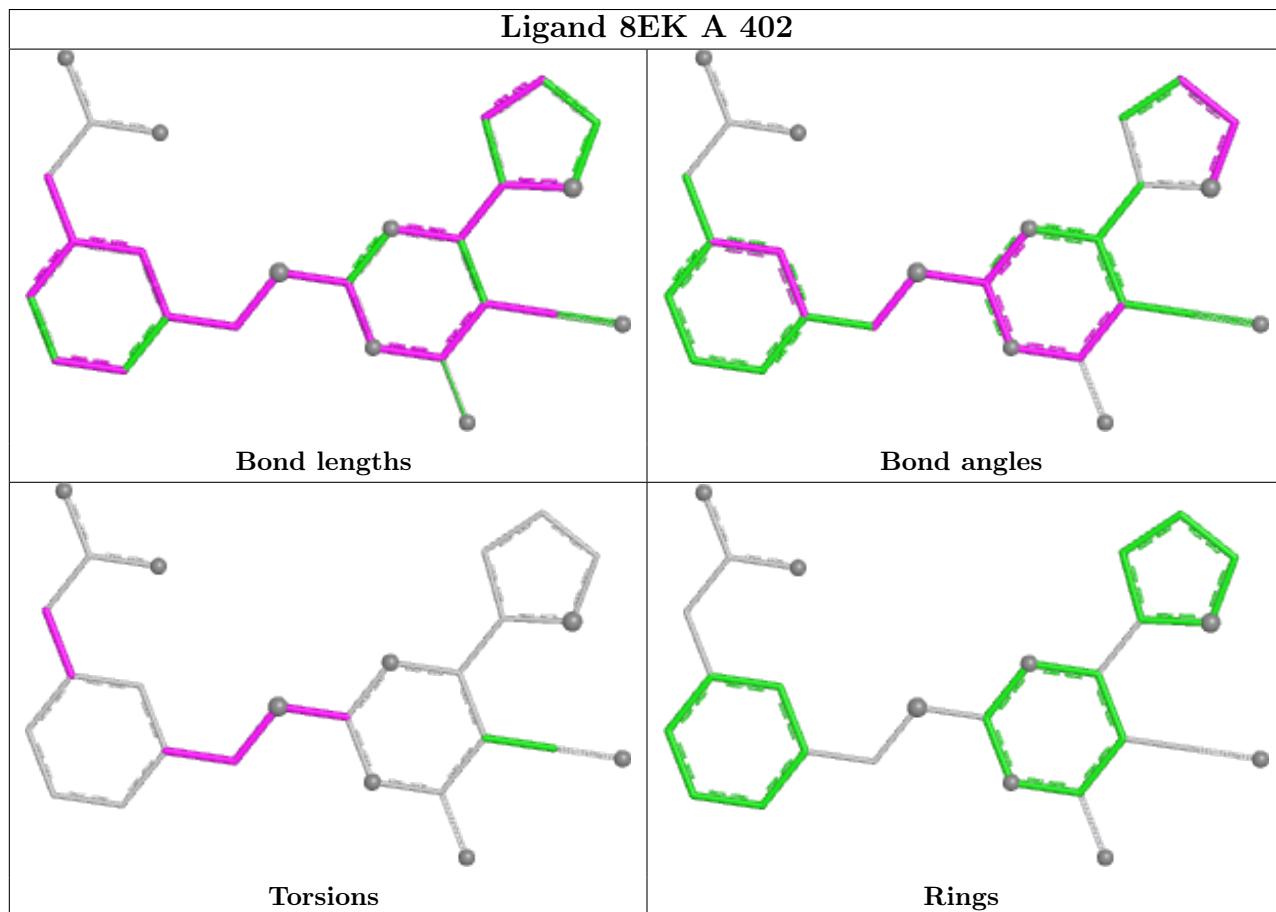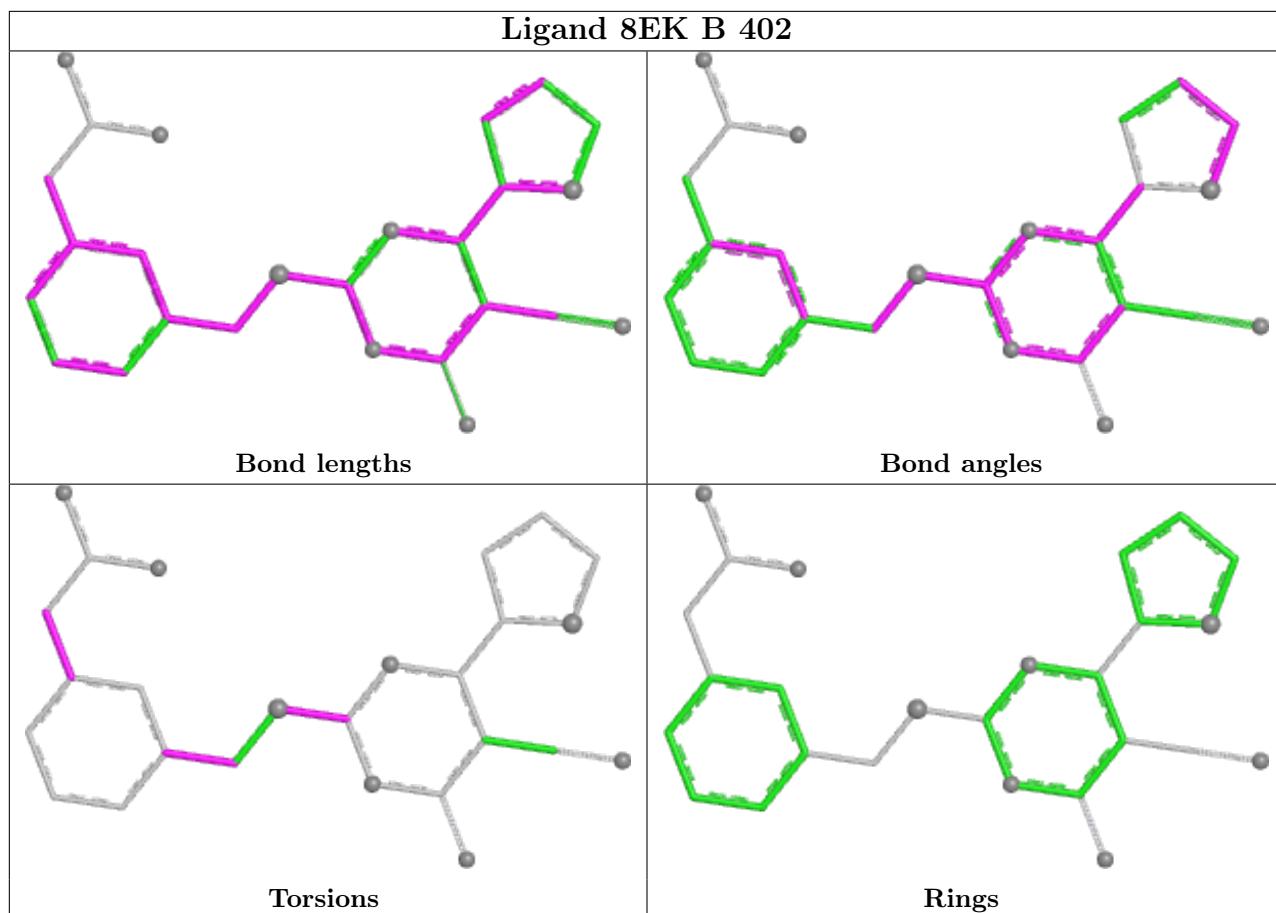
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/336 (99%)	0.43	12 (3%)	42	46	33, 50, 82, 96	0
1	B	334/336 (99%)	0.33	12 (3%)	42	46	34, 54, 83, 103	0
1	C	301/336 (89%)	0.70	32 (10%)	6	5	57, 78, 98, 119	0
1	D	320/336 (95%)	0.67	32 (10%)	7	6	54, 81, 108, 124	0
All	All	1289/1344 (95%)	0.53	88 (6%)	17	17	33, 68, 99, 124	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	46	PHE	7.4
1	D	240	PHE	6.2
1	C	176	TRP	5.1
1	C	111	PHE	5.1
1	A	249	GLN	4.7
1	C	24	GLY	4.4
1	D	255	PRO	4.3
1	D	32	HIS	4.2
1	D	254	ASN	4.1
1	A	248	ALA	4.1
1	D	188	TRP	3.9
1	C	27	VAL	3.9
1	A	251	ASN	3.9
1	A	29	LEU	3.8
1	C	191	TRP	3.8
1	D	25	GLY	3.7
1	D	256	LYS	3.7
1	C	19	LYS	3.6
1	C	80	PHE	3.6
1	C	41	LYS	3.5
1	C	53	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	36	GLU	3.4
1	C	193	VAL	3.3
1	C	188	TRP	3.3
1	B	36	GLU	3.3
1	D	180	MET	3.3
1	B	176	TRP	3.2
1	B	43	GLY	3.1
1	C	23	TYR	3.1
1	B	50	ARG	3.1
1	D	29	LEU	3.0
1	D	31	HIS	2.9
1	C	141	VAL	2.9
1	A	247	CYS	2.9
1	C	28	GLN	2.9
1	A	159	PRO	2.9
1	C	84	ALA	2.8
1	D	176	TRP	2.8
1	D	258	TYR	2.8
1	C	240	PHE	2.8
1	C	108	PRO	2.8
1	C	187	TYR	2.7
1	D	15	PRO	2.7
1	D	68	VAL	2.7
1	D	150	TRP	2.7
1	B	46	PHE	2.7
1	B	335	PHE	2.7
1	C	190	PRO	2.7
1	C	81	SER	2.7
1	D	191	TRP	2.7
1	D	149	GLU	2.6
1	D	105	VAL	2.6
1	D	81	SER	2.6
1	A	123	GLU	2.6
1	A	196	PRO	2.5
1	D	35	GLY	2.5
1	B	47	ARG	2.5
1	D	259	LEU	2.4
1	D	18	LYS	2.4
1	D	13	GLU	2.3
1	A	223	ALA	2.3
1	C	238	HIS	2.3
1	D	201	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	294	PHE	2.3
1	C	317	ASN	2.3
1	D	40	LEU	2.3
1	C	26	TRP	2.3
1	A	228	ALA	2.2
1	D	297	GLY	2.2
1	C	151	ASP	2.2
1	A	244	PRO	2.2
1	D	28	GLN	2.2
1	A	33	SER	2.2
1	B	199	THR	2.2
1	B	40	LEU	2.2
1	C	138	PHE	2.1
1	D	257	LYS	2.1
1	D	208	MET	2.1
1	B	45	VAL	2.1
1	C	58	VAL	2.1
1	C	171	LEU	2.1
1	D	144	GLY	2.1
1	B	26	TRP	2.1
1	C	54	TRP	2.0
1	C	79	MET	2.0
1	B	27	VAL	2.0
1	D	262	PHE	2.0
1	C	177	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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
4	K	A	404	1/1	0.80	0.13	70,70,70,70	0
3	8EK	B	402	26/26	0.83	0.28	59,84,97,100	26
3	8EK	A	402	26/26	0.87	0.23	47,72,81,83	0
4	K	B	404	1/1	0.90	0.28	81,81,81,81	0
4	K	A	403	1/1	0.93	0.14	56,56,56,56	0
4	K	D	402	1/1	0.93	0.08	82,82,82,82	0
4	K	B	403	1/1	0.94	0.08	55,55,55,55	0
4	K	C	402	1/1	0.96	0.07	79,79,79,79	0
2	ZN	C	401	1/1	0.96	0.09	66,66,66,66	0
2	ZN	B	401	1/1	0.97	0.15	49,49,49,49	0
2	ZN	A	401	1/1	0.98	0.17	43,43,43,43	0
2	ZN	D	401	1/1	0.98	0.17	63,63,63,63	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 8EK B 402:

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

Electron density around 8EK A 402:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.