



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:32 AM UTC

PDB ID : 6RFX / pdb_00006rfx
Title : Crystal structure of Eis2 from Mycobacterium abscessus
Authors : Blaise, M.; Kremer, L.; Olieric, V.; Alsarraf, H.; Ung, K.L.
Deposited on : 2019-04-16
Resolution : 1.90 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

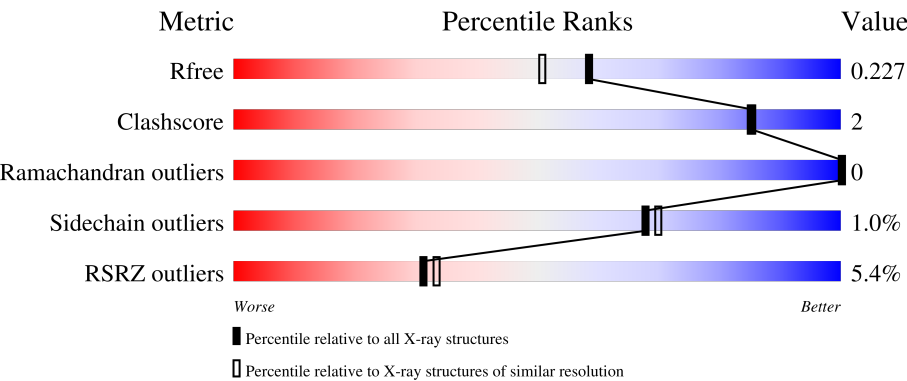
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	411	2% 94% 7% 1% 0%
1	B	411	4% 90% 7% 1% 0%
1	C	411	3% 94% 7% 1% 0%
1	D	411	2% 93% 5% 1% 0%
1	E	411	6% 91% 7% 1% 0%

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Mol	Chain	Length	Quality of chain
1	F	411	14% 92% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20624 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 Eis2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	401	Total	C	N	O	S	Se	0	0	0
			3114	1961	547	596	2	8			
1	A	404	Total	C	N	O	S	Se	0	1	0
			3133	1973	550	600	2	8			
1	B	404	Total	C	N	O	S	Se	0	1	0
			3143	1981	550	602	2	8			
1	C	403	Total	C	N	O	S	Se	0	1	0
			3128	1970	549	599	2	8			
1	E	406	Total	C	N	O	S	Se	0	0	0
			3151	1986	552	603	2	8			
1	F	406	Total	C	N	O	S	Se	0	0	0
			3151	1986	552	603	2	8			

There are 6 discrepancies between the modelled and reference sequences:

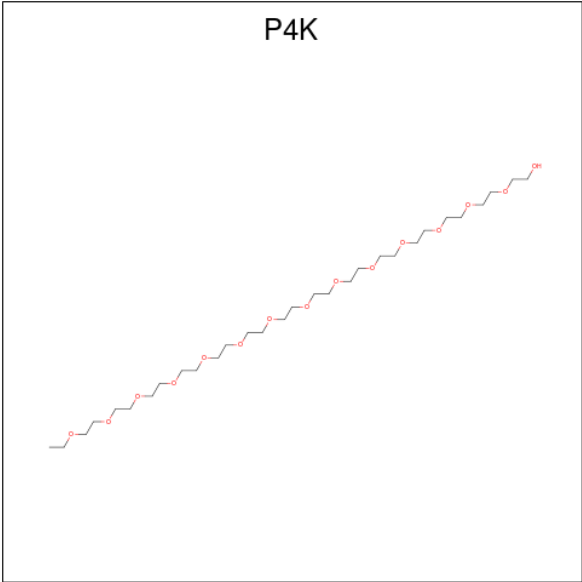
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP A0A3A1BNP8
A	1	GLY	-	expression tag	UNP A0A3A1BNP8
B	1	GLY	-	expression tag	UNP A0A3A1BNP8
C	1	GLY	-	expression tag	UNP A0A3A1BNP8
E	1	GLY	-	expression tag	UNP A0A3A1BNP8
F	1	GLY	-	expression tag	UNP A0A3A1BNP8

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is polyethylene glycol (CCD ID: P4K) (formula: $C_{30}H_{62}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			14	9	5		
3	A	1	Total	C	O	0	0
			14	9	5		
3	B	1	Total	C	O	0	0
			14	9	5		
3	B	1	Total	C	O	0	0
			14	9	5		
3	C	1	Total	C	O	0	0
			14	9	5		
3	E	1	Total	C	O	0	0
			11	7	4		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

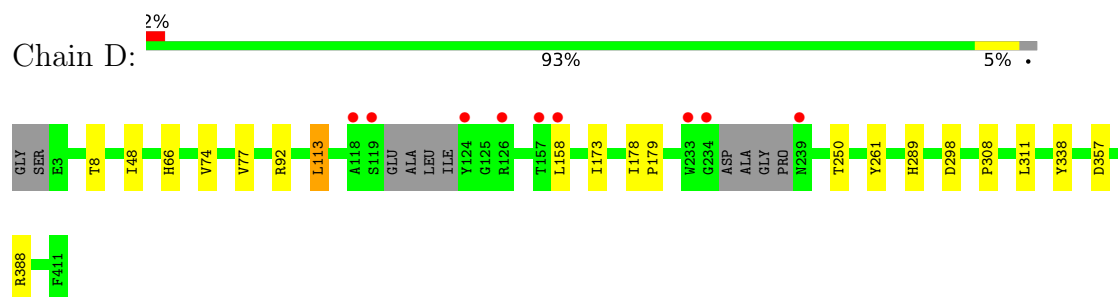
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	342	Total	O	0	0
			342	342		
5	A	328	Total	O	0	0
			328	328		
5	B	303	Total	O	0	0
			303	303		
5	C	296	Total	O	0	0
			296	296		
5	E	194	Total	O	0	0
			194	194		
5	F	151	Total	O	0	0
			151	151		

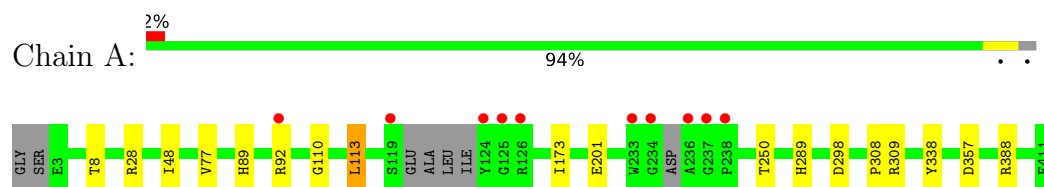
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

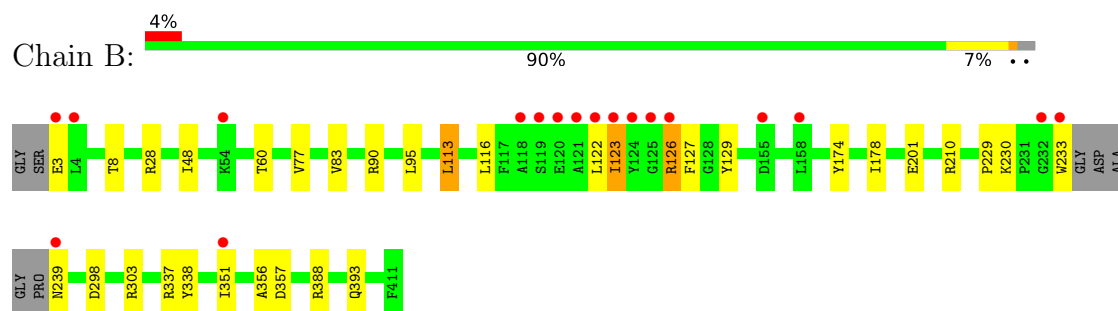
- Molecule 1: Eis2



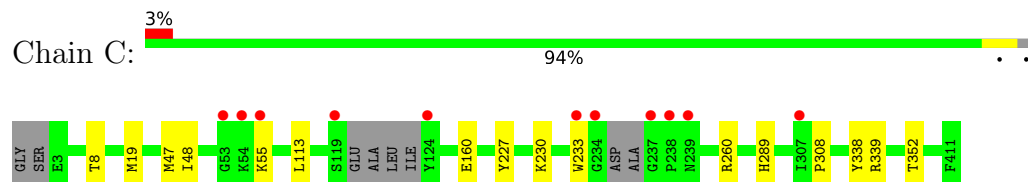
- Molecule 1: Eis2



- Molecule 1: Eis2

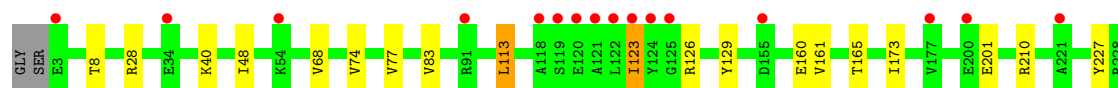


- Molecule 1: Eis2

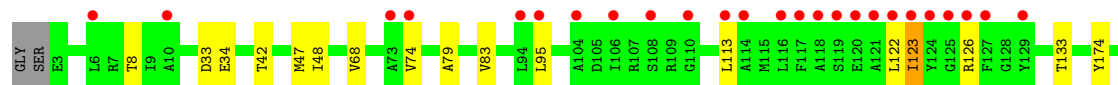
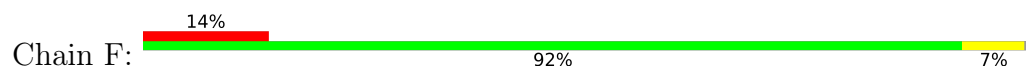


- Molecule 1: Eis2





● Molecule 1: Eis2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.45Å 79.80Å 152.68Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	49.60 – 1.90 49.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.60-1.90) 99.0 (49.60-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.15rc3_3435: ???)	Depositor
R, R_{free}	0.202 , 0.226 0.203 , 0.227	Depositor DCC
R_{free} test set	10545 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20624	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, ACT, P4K

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	0.12	0/3195	0.31	0/4329
1	B	0.14	0/3205	0.36	0/4344
1	C	0.12	0/3190	0.31	0/4322
1	D	0.12	0/3172	0.33	0/4297
1	E	0.11	0/3211	0.32	0/4352
1	F	0.11	0/3211	0.31	0/4352
All	All	0.12	0/19184	0.32	0/25996

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3133	0	3066	11	0
1	B	3143	0	3082	22	0
1	C	3128	0	3061	9	0
1	D	3114	0	3046	11	0
1	E	3151	0	3088	18	0
1	F	3151	0	3088	16	0
2	A	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	14	0	0	0	0
3	D	11	0	0	0	0
3	E	11	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
4	E	4	0	3	0	0
5	A	328	0	0	0	0
5	B	303	0	0	1	0
5	C	296	0	0	2	0
5	D	342	0	0	1	0
5	E	194	0	0	2	0
5	F	151	0	0	0	0
All	All	20624	0	18476	81	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 2.

All (81) 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:116:LEU:HD21	1:B:123:ILE:HG13	1.56	0.86
1:F:42:THR:HG23	1:F:47:MSE:HE3	1.70	0.72
1:B:60:THR:HG23	1:B:83:VAL:HG22	1.73	0.70
1:F:95:LEU:HD21	1:F:123:ILE:HG22	1.71	0.70
1:A:110:GLY:O	1:A:309:ARG:NH2	2.25	0.70
1:A:28:ARG:NH2	1:A:201:GLU:OE1	2.31	0.63
1:C:260:ARG:NH1	5:C:602:HOH:O	2.34	0.60
1:A:8:THR:HG22	1:A:48:ILE:HG22	1.84	0.58
1:B:3:GLU:N	5:B:605:HOH:O	2.35	0.58
1:C:308:PRO:HG3	1:C:338:TYR:CE1	2.40	0.56
1:E:123:ILE:HD13	1:E:123:ILE:H	1.70	0.56
1:E:40:LYS:NZ	5:E:603:HOH:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:ILE:HG13	1:F:179:PRO:HD3	1.89	0.54
1:A:77:VAL:HG23	1:A:113:LEU:HD13	1.90	0.53
1:B:8:THR:HG22	1:B:48:ILE:HG22	1.90	0.53
1:A:89:HIS:HA	1:A:92:ARG:NH1	2.23	0.53
1:B:77:VAL:HG23	1:B:113:LEU:HD13	1.90	0.53
1:B:126:ARG:HB2	1:B:127:PHE:CD2	2.44	0.53
1:D:8:THR:HG22	1:D:48:ILE:HG22	1.91	0.52
1:B:123:ILE:HD13	1:B:123:ILE:H	1.74	0.52
1:B:116:LEU:CD2	1:B:123:ILE:HG13	2.33	0.51
1:F:83:VAL:HG11	1:F:123:ILE:HD12	1.91	0.51
1:E:402:PRO:HG2	1:F:393:GLN:HG3	1.93	0.51
1:B:95:LEU:HD22	1:B:122:LEU:HD23	1.91	0.51
1:D:173:ILE:HG23	1:D:250:THR:HG23	1.93	0.51
1:A:89:HIS:HA	1:A:92:ARG:HH11	1.77	0.50
1:C:8:THR:HG22	1:C:48:ILE:HG22	1.93	0.49
1:D:92:ARG:NH1	5:D:601:HOH:O	2.36	0.49
1:F:123:ILE:HD13	1:F:123:ILE:H	1.77	0.49
1:D:308:PRO:HG3	1:D:338:TYR:CE1	2.48	0.49
1:D:77:VAL:HG23	1:D:113:LEU:HD13	1.95	0.49
1:E:83:VAL:HG11	1:E:123:ILE:HD12	1.95	0.49
1:A:308:PRO:HG3	1:A:338:TYR:CE1	2.48	0.48
1:B:298:ASP:OD2	1:C:289:HIS:HB2	2.14	0.48
1:F:68:VAL:HG22	1:F:74:VAL:HG22	1.96	0.47
1:E:298:ASP:OD2	1:F:289:HIS:HB2	2.14	0.47
1:B:210:ARG:HD3	1:B:229:PRO:HD3	1.97	0.47
1:B:337:ARG:HD3	1:B:356:ALA:HB2	1.97	0.47
1:C:19:MSE:HE1	1:C:47:MSE:HE2	1.97	0.47
1:D:178:ILE:HG13	1:D:179:PRO:HD3	1.97	0.47
1:F:308:PRO:HG3	1:F:338:TYR:CE2	2.50	0.46
1:F:8:THR:HG22	1:F:48:ILE:HG22	1.97	0.45
1:D:66:HIS:HB3	1:D:74:VAL:HG12	1.99	0.45
1:D:289:HIS:HB2	1:A:298:ASP:OD2	2.16	0.45
1:D:298:ASP:OD2	1:A:289:HIS:HB2	2.17	0.45
1:E:68:VAL:HG22	1:E:74:VAL:HG22	1.98	0.45
1:B:28:ARG:NH2	1:B:201:GLU:OE1	2.49	0.45
1:A:173:ILE:HG23	1:A:250:THR:HG23	1.98	0.44
1:E:210:ARG:NH1	5:E:612:HOH:O	2.50	0.44
1:B:357:ASP:OD1	1:B:388:ARG:HD3	2.17	0.44
1:E:160:GLU:OE2	1:E:227:TYR:OH	2.34	0.44
1:B:174:TYR:CZ	1:B:178:ILE:HG21	2.53	0.44
1:D:357:ASP:OD1	1:D:388:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:TYR:CZ	1:F:178:ILE:HG21	2.53	0.44
1:E:161:VAL:HB	1:E:165:THR:HB	2.01	0.43
1:B:83:VAL:HG11	1:B:123:ILE:HD12	1.99	0.43
1:A:357:ASP:OD1	1:A:388:ARG:HD3	2.19	0.43
1:C:339:ARG:HB2	1:C:352:THR:HG21	2.00	0.43
1:E:77:VAL:HG23	1:E:113:LEU:HD13	2.00	0.43
1:E:129:TYR:CE2	1:E:303:ARG:HB2	2.54	0.43
1:E:230:LYS:HE3	1:E:233:TRP:CZ3	2.54	0.43
1:C:260:ARG:HD3	5:C:867:HOH:O	2.18	0.43
1:E:173:ILE:HG23	1:E:250:THR:HG23	2.00	0.42
1:E:241:GLU:HG2	1:E:270:LYS:HB3	2.00	0.42
1:F:241:GLU:HG2	1:F:270:LYS:HB3	2.02	0.42
1:B:123:ILE:H	1:B:123:ILE:CD1	2.32	0.42
1:B:90:ARG:CZ	1:B:122:LEU:HD11	2.50	0.42
1:E:8:THR:HG22	1:E:48:ILE:HG22	2.02	0.41
1:B:129:TYR:CE2	1:B:303:ARG:HB2	2.55	0.41
1:B:230:LYS:HE3	1:B:233:TRP:CZ3	2.55	0.41
1:F:33:ASP:OD1	1:F:34:GLU:N	2.53	0.41
1:E:28:ARG:NH2	1:E:201:GLU:OE1	2.53	0.41
1:E:210:ARG:HD3	1:E:229:PRO:HD3	2.01	0.41
1:B:116:LEU:HD21	1:B:123:ILE:CG1	2.39	0.41
1:B:338:TYR:CE2	1:B:351:ILE:HG12	2.56	0.41
1:D:158:LEU:HD11	1:D:261:TYR:CD1	2.56	0.41
1:F:133:THR:HB	1:F:300:ILE:HB	2.03	0.40
1:C:160:GLU:OE2	1:C:227:TYR:OH	2.39	0.40
1:F:79:ALA:HB1	1:F:411:PHE:CD1	2.56	0.40
1:C:230:LYS:HE3	1:C:233:TRP:CZ3	2.56	0.40
1:E:289:HIS:HB2	1:F:298:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/411 (97%)	392 (98%)	7 (2%)	0	100	100
1	B	401/411 (98%)	392 (98%)	9 (2%)	0	100	100
1	C	398/411 (97%)	393 (99%)	5 (1%)	0	100	100
1	D	395/411 (96%)	388 (98%)	7 (2%)	0	100	100
1	E	402/411 (98%)	392 (98%)	10 (2%)	0	100	100
1	F	402/411 (98%)	392 (98%)	10 (2%)	0	100	100
All	All	2397/2466 (97%)	2349 (98%)	48 (2%)	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	328/324 (101%)	327 (100%)	1 (0%)	86	88
1	B	330/324 (102%)	325 (98%)	5 (2%)	57	56
1	C	328/324 (101%)	326 (99%)	2 (1%)	78	81
1	D	326/324 (101%)	324 (99%)	2 (1%)	78	81
1	E	330/324 (102%)	326 (99%)	4 (1%)	63	63
1	F	330/324 (102%)	325 (98%)	5 (2%)	57	56
All	All	1972/1944 (101%)	1953 (99%)	19 (1%)	68	70

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	LEU
1	D	311	LEU
1	A	113	LEU
1	B	113	LEU
1	B	123	ILE
1	B	126	ARG
1	B	239	ASN

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Mol	Chain	Res	Type
1	B	393	GLN
1	C	55	LYS
1	C	113	LEU
1	E	113	LEU
1	E	123	ILE
1	E	126	ARG
1	E	311	LEU
1	F	113	LEU
1	F	122	LEU
1	F	123	ILE
1	F	126	ARG
1	F	210	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	239	ASN
1	D	274	HIS
1	A	102	GLN
1	B	239	ASN
1	B	288	ASN
1	B	393	GLN
1	C	346	HIS
1	E	102	GLN
1	E	288	ASN
1	F	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 ligands are modelled in this entry.

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	P4K	D	502	-	10,10,44	0.52	0	9,9,43	0.24	0
3	P4K	B	502	-	13,13,44	0.53	0	12,12,43	0.21	0
3	P4K	B	504	-	13,13,44	0.53	0	12,12,43	0.20	0
4	ACT	D	503	-	3,3,3	0.77	0	3,3,3	0.91	0
2	CIT	F	501	-	12,12,12	1.50	1 (8%)	17,17,17	1.82	4 (23%)
3	P4K	C	502	-	13,13,44	0.53	0	12,12,43	0.20	0
4	ACT	B	503	-	3,3,3	0.77	0	3,3,3	0.94	0
4	ACT	A	503	-	3,3,3	0.78	0	3,3,3	0.91	0
2	CIT	B	501	-	12,12,12	1.52	1 (8%)	17,17,17	1.82	4 (23%)
4	ACT	C	503	-	3,3,3	0.78	0	3,3,3	0.87	0
2	CIT	A	501	-	12,12,12	1.36	1 (8%)	17,17,17	0.98	2 (11%)
3	P4K	A	502	-	13,13,44	0.53	0	12,12,43	0.19	0
3	P4K	A	504	-	13,13,44	0.53	0	12,12,43	0.16	0
2	CIT	C	501	-	12,12,12	1.41	1 (8%)	17,17,17	0.99	2 (11%)
3	P4K	E	502	-	10,10,44	0.52	0	9,9,43	0.19	0
2	CIT	E	501	-	12,12,12	1.29	1 (8%)	17,17,17	0.45	0
4	ACT	E	503	-	3,3,3	0.76	0	3,3,3	0.91	0
2	CIT	D	501	-	12,12,12	1.54	1 (8%)	17,17,17	2.02	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
3	P4K	D	502	-	-	6/8/8/42	-
3	P4K	B	502	-	-	7/11/11/42	-
3	P4K	B	504	-	-	7/11/11/42	-
2	CIT	F	501	-	-	6/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P4K	C	502	-	-	4/11/11/42	-
2	CIT	B	501	-	-	0/16/16/16	-
2	CIT	A	501	-	-	0/16/16/16	-
3	P4K	A	502	-	-	6/11/11/42	-
3	P4K	A	504	-	-	8/11/11/42	-
2	CIT	C	501	-	-	0/16/16/16	-
3	P4K	E	502	-	-	5/8/8/42	-
2	CIT	E	501	-	-	0/16/16/16	-
2	CIT	D	501	-	-	0/16/16/16	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	CIT	C3-C6	3.36	1.57	1.53
2	E	501	CIT	C3-C6	3.36	1.57	1.53
2	B	501	CIT	C3-C6	3.26	1.56	1.53
2	F	501	CIT	C3-C6	3.10	1.56	1.53
2	A	501	CIT	C3-C6	3.06	1.56	1.53
2	D	501	CIT	C3-C6	2.90	1.56	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	CIT	O6-C6-C3	4.77	122.29	113.14
2	D	501	CIT	O6-C6-C3	4.74	122.24	113.14
2	F	501	CIT	O6-C6-C3	4.73	122.20	113.14
2	D	501	CIT	O5-C6-C3	-4.30	113.76	122.09
2	B	501	CIT	O5-C6-C3	-4.26	113.84	122.09
2	F	501	CIT	O5-C6-C3	-4.22	113.92	122.09
2	D	501	CIT	O2-C1-C2	2.63	122.66	114.35
2	A	501	CIT	O4-C5-C4	2.58	122.54	114.35
2	C	501	CIT	O4-C5-C4	2.58	122.53	114.35
2	D	501	CIT	O1-C1-C2	-2.58	115.65	122.95
2	F	501	CIT	O2-C1-C2	2.55	122.43	114.35
2	D	501	CIT	O4-C5-C4	2.52	122.34	114.35
2	B	501	CIT	O2-C1-C2	2.51	122.30	114.35
2	A	501	CIT	O3-C5-C4	-2.50	115.87	122.95
2	C	501	CIT	O3-C5-C4	-2.49	115.90	122.95
2	F	501	CIT	O1-C1-C2	-2.47	115.96	122.95
2	B	501	CIT	O1-C1-C2	-2.44	116.05	122.95
2	D	501	CIT	O3-C5-C4	-2.43	116.07	122.95

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	P4K	O4-C7-C8-O5
3	B	504	P4K	O2-C3-C4-O3
3	E	502	P4K	O3-C5-C6-O4
3	A	504	P4K	O2-C3-C4-O3
3	A	504	P4K	O3-C5-C6-O4
3	D	502	P4K	O3-C5-C6-O4
3	B	504	P4K	O3-C5-C6-O4
3	D	502	P4K	O4-C7-C8-O5
3	E	502	P4K	O6-C10-C9-O5
3	A	502	P4K	O2-C3-C4-O3
3	A	504	P4K	O6-C10-C9-O5
3	B	504	P4K	O6-C10-C9-O5
3	A	502	P4K	C7-C8-O5-C9
3	B	502	P4K	O6-C10-C9-O5
3	D	502	P4K	C7-C8-O5-C9
3	C	502	P4K	O6-C10-C9-O5
3	D	502	P4K	C8-C7-O4-C6
3	B	502	P4K	C8-C7-O4-C6
3	E	502	P4K	C8-C7-O4-C6
3	C	502	P4K	C7-C8-O5-C9
3	B	504	P4K	C3-C4-O3-C5
3	A	504	P4K	C7-C8-O5-C9
3	E	502	P4K	C7-C8-O5-C9
3	A	502	P4K	C8-C7-O4-C6
3	B	502	P4K	C7-C8-O5-C9
3	A	504	P4K	C6-C5-O3-C4
3	B	504	P4K	C4-C3-O2-C2
3	E	502	P4K	C5-C6-O4-C7
3	D	502	P4K	C5-C6-O4-C7
3	B	504	P4K	C6-C5-O3-C4
3	D	502	P4K	O6-C10-C9-O5
3	B	502	P4K	C10-C9-O5-C8
3	C	502	P4K	O4-C7-C8-O5
3	B	502	P4K	O2-C3-C4-O3
3	A	504	P4K	C4-C3-O2-C2
2	F	501	CIT	C2-C3-C6-O5
2	F	501	CIT	C2-C3-C6-O6
2	F	501	CIT	C4-C3-C6-O5
3	B	502	P4K	O3-C5-C6-O4
3	C	502	P4K	C8-C7-O4-C6

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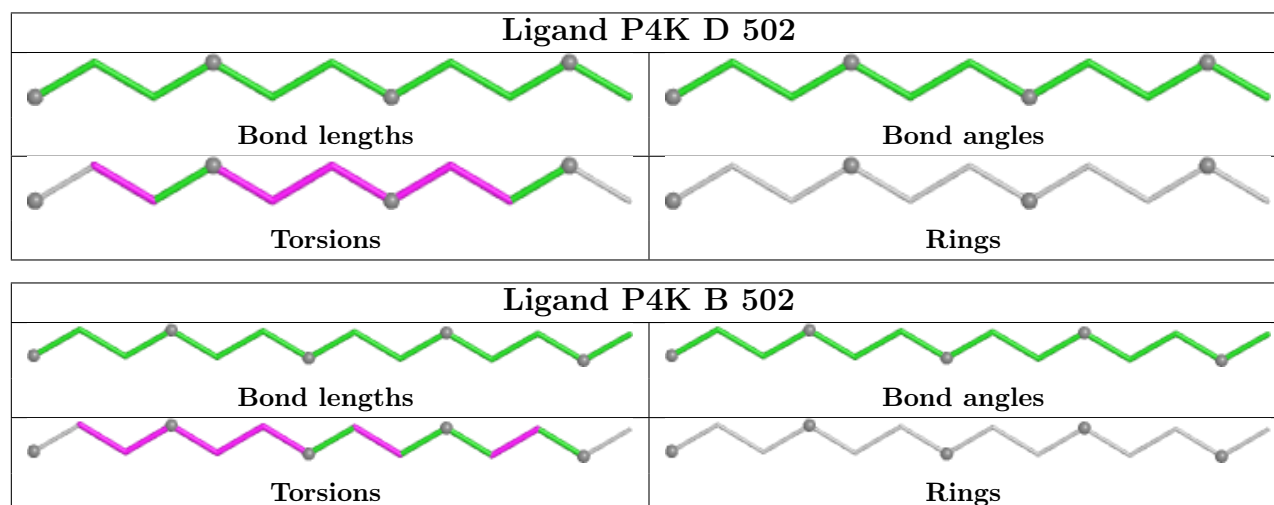
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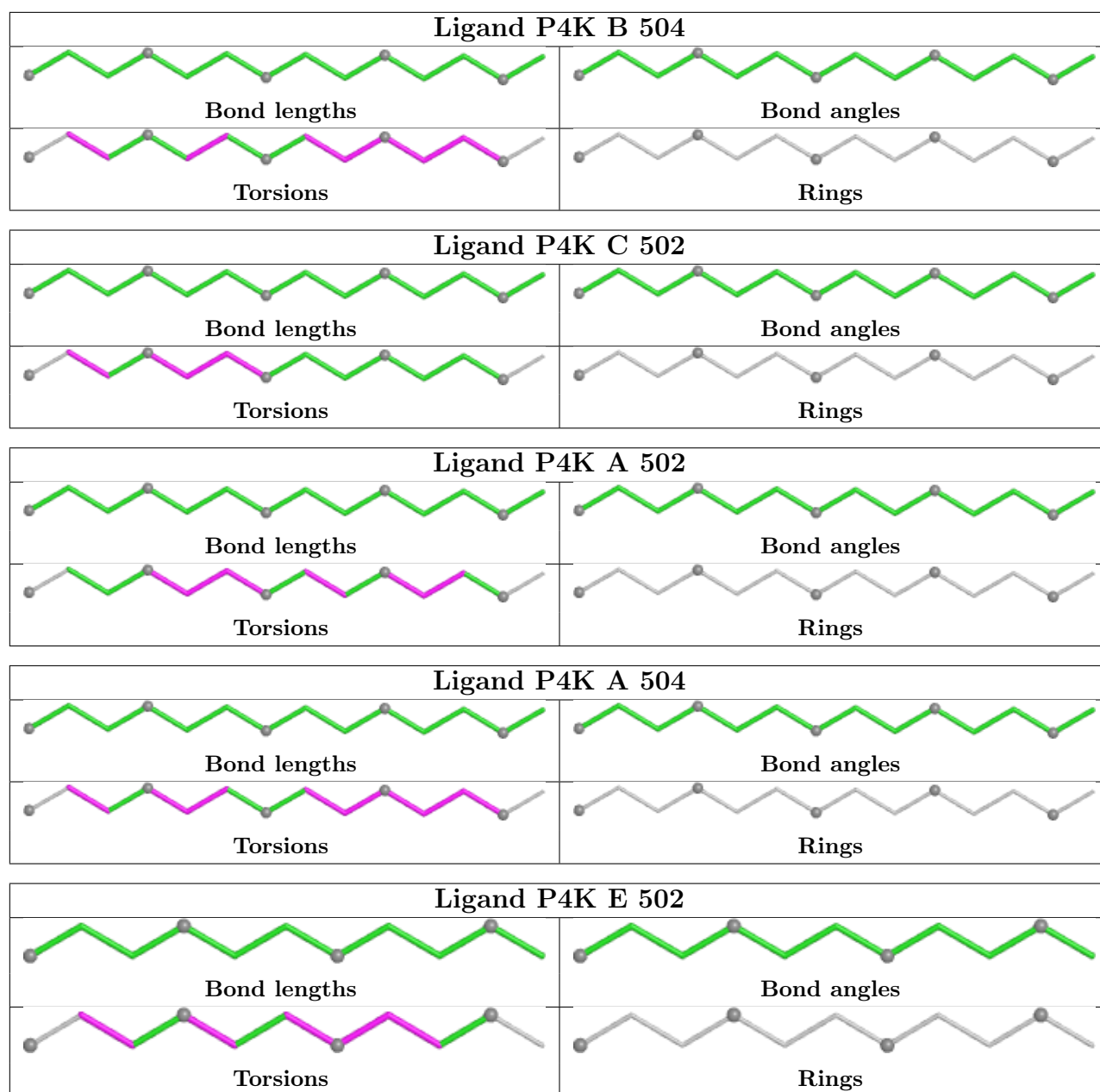
Mol	Chain	Res	Type	Atoms
3	A	502	P4K	O3-C5-C6-O4
3	A	504	P4K	C3-C4-O3-C5
2	F	501	CIT	C4-C3-C6-O6
3	A	502	P4K	C3-C4-O3-C5
3	B	502	P4K	O4-C7-C8-O5
3	B	504	P4K	O4-C7-C8-O5
2	F	501	CIT	C1-C2-C3-C6
2	F	501	CIT	C1-C2-C3-O7
3	A	502	P4K	O4-C7-C8-O5

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 ⓘ

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	396/411 (96%)	0.17	10 (2%) 58 62	20, 36, 55, 81	1 (0%)
1	B	396/411 (96%)	0.22	18 (4%) 38 40	22, 36, 59, 73	1 (0%)
1	C	395/411 (96%)	0.24	11 (2%) 55 59	18, 41, 62, 77	1 (0%)
1	D	393/411 (95%)	0.07	9 (2%) 61 65	19, 34, 57, 83	0
1	E	398/411 (96%)	0.63	23 (5%) 29 30	28, 48, 66, 86	0
1	F	398/411 (96%)	1.14	57 (14%) 6 6	33, 59, 78, 94	0
All	All	2376/2466 (96%)	0.41	128 (5%) 31 33	18, 42, 69, 94	3 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	ILE	6.0
1	A	124	TYR	4.9
1	D	124	TYR	4.8
1	E	122	LEU	4.8
1	B	121	ALA	4.8
1	B	119	SER	4.7
1	F	122	LEU	4.7
1	F	121	ALA	4.6
1	F	123	ILE	4.6
1	D	158	LEU	4.2
1	B	122	LEU	4.2
1	B	233	TRP	4.2
1	A	236	ALA	4.1
1	F	120	GLU	4.0
1	F	238	PRO	3.9
1	E	238	PRO	3.8
1	F	353	THR	3.8
1	E	233	TRP	3.8
1	C	124	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	120	GLU	3.7
1	F	351	ILE	3.7
1	B	124	TYR	3.6
1	A	119	SER	3.5
1	B	125	GLY	3.5
1	D	233	TRP	3.4
1	F	233	TRP	3.4
1	D	234	GLY	3.3
1	B	118	ALA	3.3
1	A	238	PRO	3.3
1	F	119	SER	3.3
1	E	123	ILE	3.2
1	E	234	GLY	3.2
1	D	239	ASN	3.1
1	F	106	ILE	3.1
1	F	358	ILE	3.1
1	E	125	GLY	3.1
1	B	155	ASP	3.1
1	B	351	ILE	3.0
1	F	316	TYR	3.0
1	B	126	ARG	2.9
1	F	110	GLY	2.9
1	F	338	TYR	2.9
1	C	237	GLY	2.9
1	F	125	GLY	2.9
1	B	239	ASN	2.9
1	C	233	TRP	2.9
1	E	121	ALA	2.8
1	F	117	PHE	2.8
1	E	239	ASN	2.8
1	C	234	GLY	2.8
1	C	55	LYS	2.8
1	B	158	LEU	2.8
1	F	318	ALA	2.7
1	D	119	SER	2.7
1	C	119	SER	2.7
1	F	124	TYR	2.7
1	F	95	LEU	2.7
1	F	113	LEU	2.7
1	A	234	GLY	2.6
1	C	238	PRO	2.6
1	F	324	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	351	ILE	2.6
1	F	352	THR	2.6
1	F	317	ALA	2.6
1	F	347	ALA	2.5
1	F	74	VAL	2.5
1	D	126	ARG	2.5
1	A	125	GLY	2.5
1	F	234	GLY	2.5
1	F	366	GLY	2.5
1	F	73	ALA	2.5
1	F	116	LEU	2.5
1	B	54	LYS	2.5
1	E	177	VAL	2.4
1	F	118	ALA	2.4
1	A	233	TRP	2.4
1	F	387	LEU	2.4
1	F	320	VAL	2.4
1	F	186	SER	2.4
1	F	350	GLU	2.3
1	F	349	CYS	2.3
1	E	3	GLU	2.3
1	F	360	LEU	2.3
1	E	240	ALA	2.3
1	C	307	ILE	2.3
1	F	108	SER	2.3
1	E	200	GLU	2.3
1	F	340	LEU	2.3
1	D	118	ALA	2.2
1	F	10	ALA	2.2
1	E	119	SER	2.2
1	C	239	ASN	2.2
1	F	239	ASN	2.2
1	D	157	THR	2.2
1	A	126	ARG	2.2
1	F	367	SER	2.2
1	B	4	LEU	2.2
1	F	94	LEU	2.2
1	F	104	ALA	2.2
1	F	393	GLN	2.2
1	C	53	GLY	2.2
1	F	126	ARG	2.2
1	F	127	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	155	ASP	2.1
1	F	345	ASP	2.1
1	B	3	GLU	2.1
1	F	205	GLU	2.1
1	E	221	ALA	2.1
1	F	114	ALA	2.1
1	E	124	TYR	2.1
1	F	307	ILE	2.1
1	A	92	ARG	2.1
1	B	232	GLY	2.1
1	C	54	LYS	2.1
1	E	54	LYS	2.1
1	E	34	GLU	2.1
1	F	6	LEU	2.1
1	E	118	ALA	2.1
1	F	341	ARG	2.1
1	A	237	GLY	2.1
1	F	392	VAL	2.1
1	E	91	ARG	2.1
1	B	120	GLU	2.0
1	F	129	TYR	2.0
1	F	322	VAL	2.0
1	F	312	ALA	2.0
1	E	266	ASP	2.0
1	F	308	PRO	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

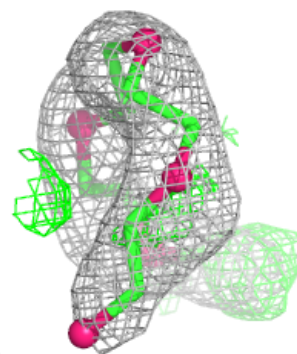
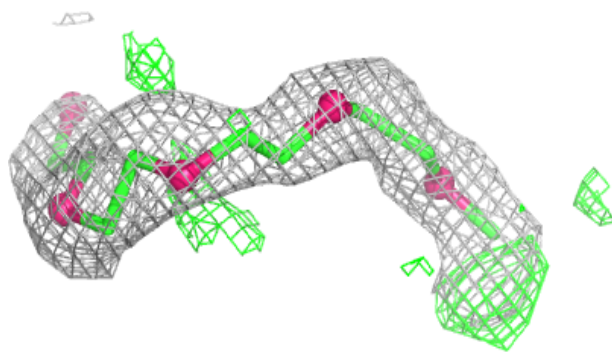
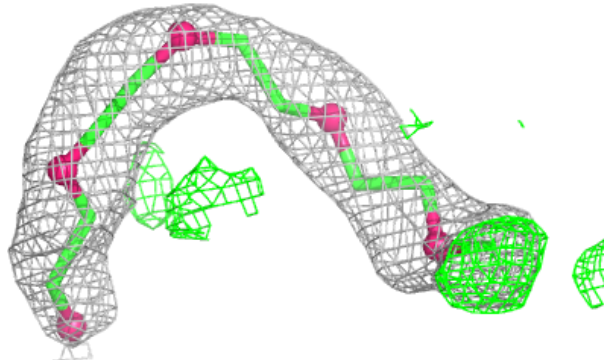
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P4K	A	502	14/45	0.74	0.19	56,61,68,69	0
3	P4K	A	504	14/45	0.76	0.23	54,61,72,74	0
2	CIT	F	501	13/13	0.77	0.13	64,67,73,74	0
3	P4K	D	502	11/45	0.79	0.20	54,62,64,66	0
3	P4K	B	504	14/45	0.79	0.20	62,67,68,68	0
3	P4K	C	502	14/45	0.79	0.18	68,69,70,70	0
3	P4K	B	502	14/45	0.81	0.18	51,58,70,71	0
3	P4K	E	502	11/45	0.81	0.18	63,64,66,66	0
4	ACT	E	503	4/4	0.85	0.16	47,50,51,51	4
2	CIT	C	501	13/13	0.87	0.13	61,64,65,65	0
2	CIT	E	501	13/13	0.88	0.11	44,51,62,64	13
2	CIT	A	501	13/13	0.88	0.10	53,55,61,63	0
4	ACT	C	503	4/4	0.89	0.14	34,40,43,57	0
2	CIT	D	501	13/13	0.91	0.09	35,38,51,53	0
2	CIT	B	501	13/13	0.91	0.09	36,40,47,53	0
4	ACT	D	503	4/4	0.92	0.10	35,41,43,52	0
4	ACT	A	503	4/4	0.93	0.10	40,43,43,46	0
4	ACT	B	503	4/4	0.94	0.11	41,45,47,57	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.

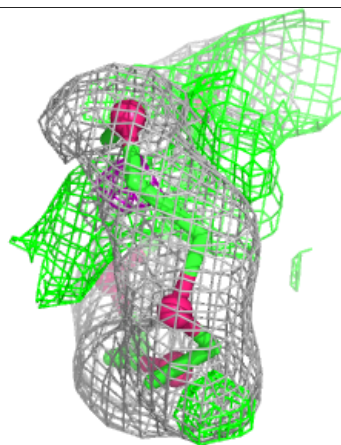
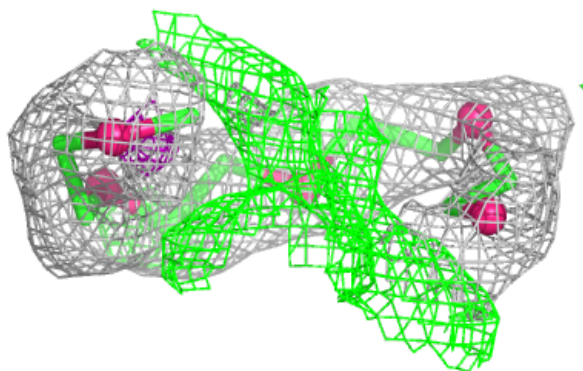
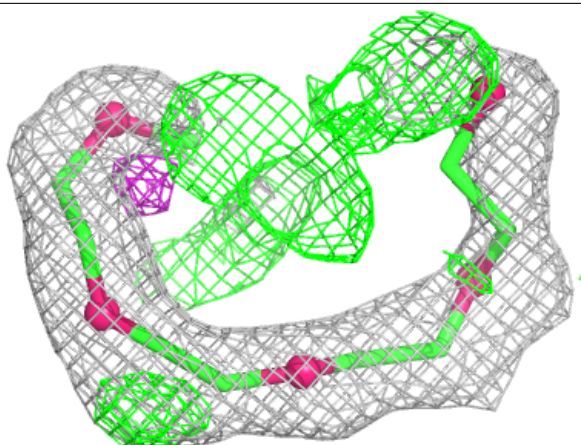
Electron density around P4K A 502:

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



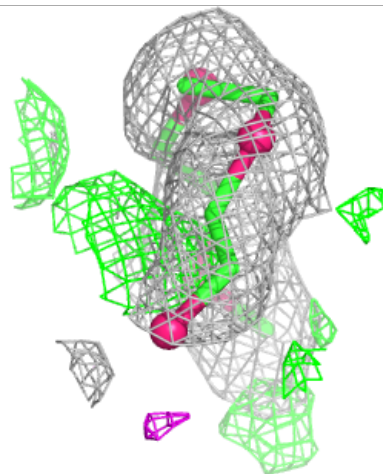
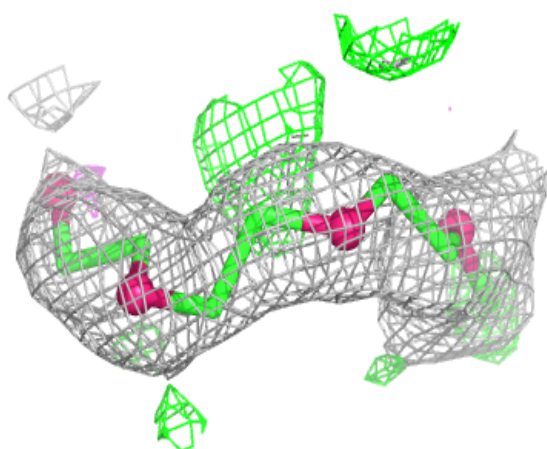
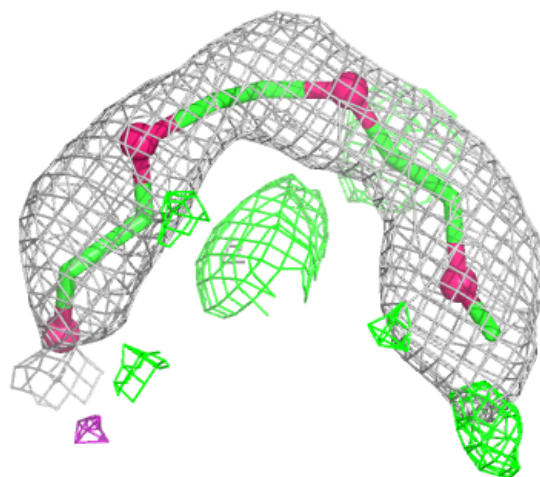
Electron density around P4K A 504:

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



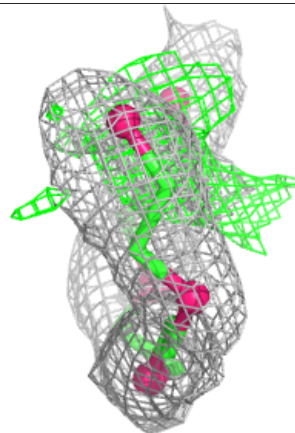
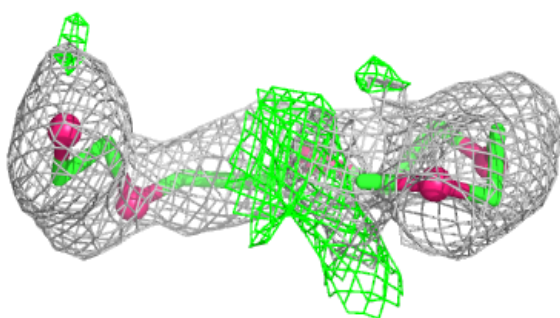
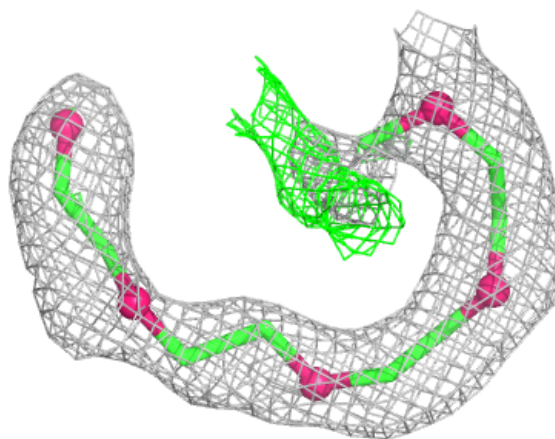
Electron density around P4K D 502:

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

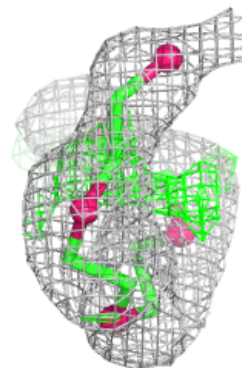
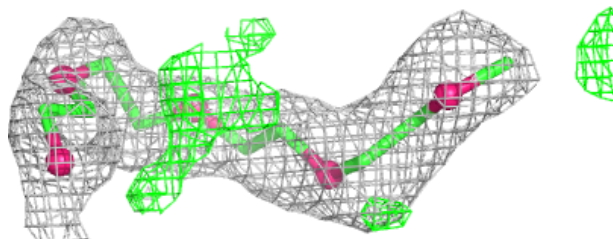
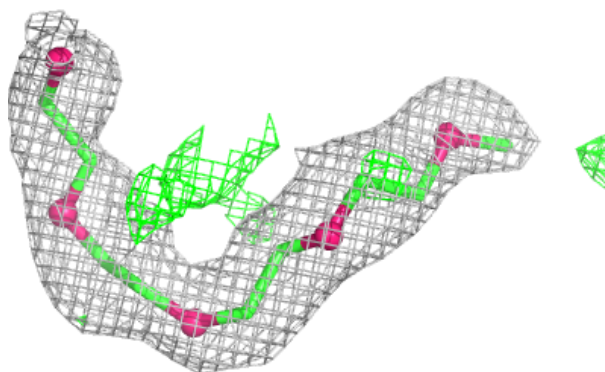


Electron density around P4K B 504:

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

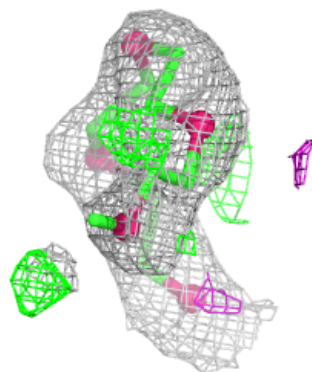
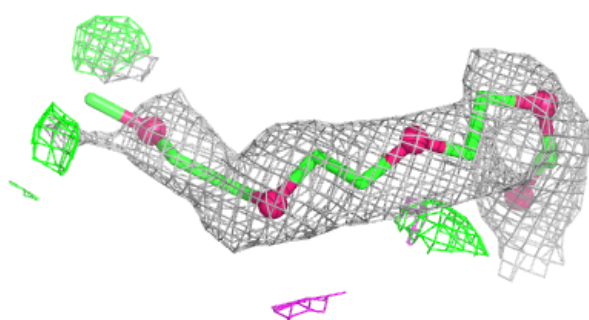
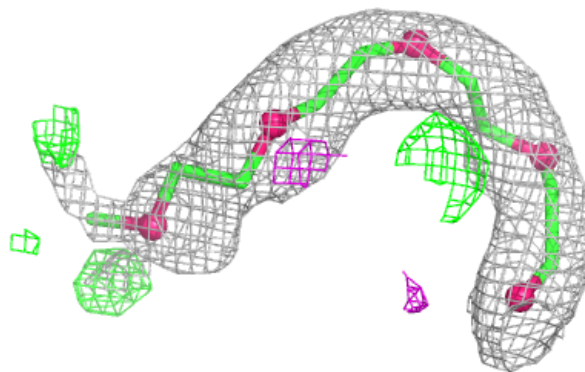
**Electron density around P4K C 502:**

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

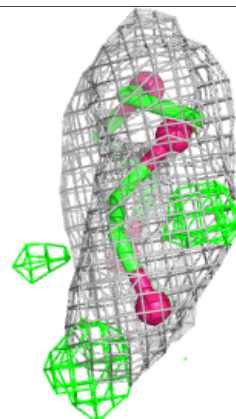
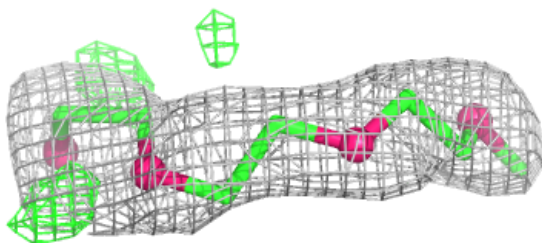
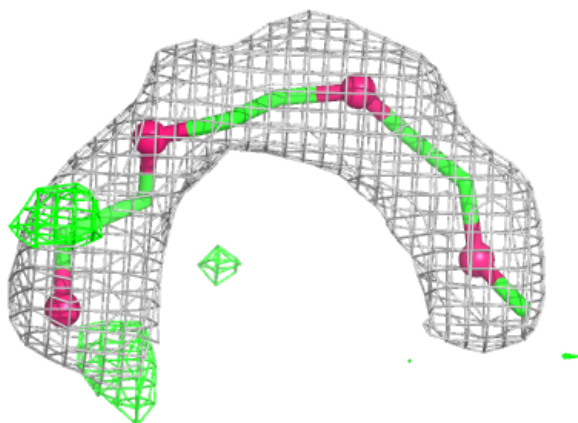


Electron density around P4K B 502:

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

**Electron density around P4K E 502:**

$2mF_o-DF_c$ (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.